A Novel Semi-Supervised Multi-Label Twin Support Vector Machine

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Abstract: Multi-label learning is a meaningful supervised learning task in which each sample may belong to multiple labels simultaneously. Due to this characteristic, multi-label learning is more complicated and more difficult than multi-class classification learning. The multi-label twin support vector machine (MLTSVM) [1], which is an effective multi-label learning algorithm based on the twin support vector machine (TSVM), has been widely studied because of its good classification performance. To obtain good generalization performance, the MLTSVM often needs a large number of labelled samples. In practical engineering problems, it is very time consuming and difficult to obtain all labels of all samples for multi-label learning problems, so we can only obtain a large number of partially labelled and unlabelled samples and a small number of labelled samples. However, the MLTSVM can use only expensive labelled samples and ignores inexpensive partially labelled and unlabelled samples. Because of the MLTSVM’s disadvantages, we propose an alternative novel semi-supervised multi-label twin support vector machine, named SS-MLTSVM, which can take full advantage of the geometric information of the edge distribution embedded in partially labelled and unlabelled samples by introducing a manifold regularization term into each sub-classifier and use the successive overrelaxation (SOR) method to speed up the solving process. Experimental results on several publicly available benchmark multi-label datasets show that, compared with the classical MLTSVM, our proposed SS-MLTSVM has better classification performance.

Keywords: Multi-label learning; semi-supervised learning; TSVM; MLTSVM

1 Introduction

Multi-label learning is a meaningful supervised learning task, wherein each sample may belong to multiple different labels simultaneously. In real life, many applications employ multi-label learning, including text classification [2,3], image annotation [4], bioinformatics [5], and so on [6]. Because the samples can have multiple labels simultaneously, multi-label learning is more complicated and more difficult than multi-class classification learning. At present, there are two kinds of methods to solve multi-label learning problems: problem transformation and algorithm adaptation. The problem transformation solves the multi-label learning problem by transforming it into one or more single-label problems, such as
binary relevance (BR) [7], classifier chains (CC) [8], label powerset (LP) [9], calibrated label ranking (CLR) [10], and random k-labelsets (RAKEL) [11]. The algorithm adaptation extends the existing single-label learning algorithm to handle multi-label learning problems, such as multi-label k-nearest neighbour (ML-kNN) [12], multi-label decision tree (ML-DT) [13], ranking support vector machine (Rank-SVM) [14], and collective multi-label classifier (CML) [15].

The TSVM [16], proposed by Jayadeva, is used to solve classification problems. It has been widely studied because of its good classification performance. Subsequent to its release, many improved algorithms have been proposed [17–29]. The aforementioned improved algorithms can solve only single-label learning problems, not multi-label learning problems. In 2016, Chen et al. extended the TSVM to solve multi-label learning problems and proposed a multi-label twin support vector machine (MLTSVM) [1]. Compared with other traditional multi-label classification algorithms, the MLTSVM has better generalization performance. Thereafter, many improved algorithms of MLTSVM have been proposed [30,31]. Hanifelou et al. introduced local information and structural information of samples into the MLTSVM and proposed the k-nearest neighbour-based MLTSVM with priority of labels (PKNN-MLTSVM) [30]. Meisam et al. proposed the structural least square twin support vector machine for multi-label learning (ML-SLSTSVM) [31], which proposed a least squares version of the MLTSVM and added structural information of samples.

The aforementioned improvements to the MLTSVM mainly focused on improving the generalization performance and learning speed. It is very time consuming and difficult to obtain all labels of all samples for multi-label learning problems; in fact, we can obtain only a large number of partially labelled and unlabelled samples and a small number of labelled samples. However, the MLTSVM and its improvements can use only expensive labelled samples and ignores inexpensive partially labelled and unlabelled samples. Because of this disadvantage, we propose a novel semi-supervised MLTSVM, named SS-MLTSVM, which can take full advantage of the geometric information of the edge distribution embedded in partially labelled and unlabelled samples by introducing a manifold regularization term into each sub-classifier and use the successive overrelaxation (SOR) method to increase the solving speed. Experimental results show that, compared with the MLTSVM, our SS-MLTSVM has better classification performance.

The structure of this paper is as follows: Section 2 introduces some related works, such as the TSVM and MLTSVM. In Section 3, the SS-MLTSVM is introduced in detail, including the linear model, nonlinear model, decision rules and training algorithm. The fourth section gives the experimental results of the proposed algorithm on the benchmark datasets. The fifth section is the conclusion.

2 Related Works

2.1 TSVM

For the binary classification problem, we suppose the training set is $T = \{(x_i, y_i) | i = 1, \ldots, m\}$, where $x_i \in \mathbb{R}^n$ is the training sample and $y_i \in \{+1, -1\}$ is the label corresponding to the training sample $x_i$. We denote positive training samples by $A \in \mathbb{R}^{m_1 \times n}$ and negative training samples by $B \in \mathbb{R}^{m_2 \times n}$. $m = m_1 + m_2$ is the total number of training samples.

The TSVM is aimed to find two nonparallel hyperplanes:

$$f_1(x) : w_1^T x + b_1 = 0, \quad f_2(x) : w_2^T x + b_2 = 0.$$  (1)
The original problem of TSVM is:
\[
\begin{align*}
\min_{w_1, b_1, \xi_1} & \quad \frac{1}{2} \|Aw_1 + e_1b_1\|^2 + c_1 \xi_1^T \xi_2 \\
\text{s.t.} & \quad -(Bw_1 + e_2b_1) + \xi_2 \geq e_2, \xi_2 \geq 0
\end{align*}
\]
(2)
\[
\begin{align*}
\min_{w_2, b_2, \xi_2} & \quad \frac{1}{2} \|Bw_2 + e_2b_2\|^2 + c_2 \xi_1^T \xi_1 \\
\text{s.t.} & \quad Aw_2 + e_1b_2 + \xi_1 \geq e_1, \xi_1 \geq 0
\end{align*}
\]
(3)
where \(c_1\) and \(c_2\) are the penalty parameters, \(\xi_1\) and \(\xi_2\) are the slack variables, and \(e_1\) and \(e_2\) are all 1 vector of the proper dimension.

By introducing the Lagrange multiplier, the dual problems of (2) and (3) can be obtained as follows:
\[
\begin{align*}
\max_{\alpha} & \quad \alpha^T \xi_2 - \frac{1}{2} \alpha^T G (H^T H)^{-1} G^T \alpha \\
\text{s.t.} & \quad 0 \leq \alpha \leq c_1 e_2
\end{align*}
\]
(4)
\[
\begin{align*}
\max_{\gamma} & \quad \gamma^T \xi_1 - \frac{1}{2} \gamma^T H (G^T G)^{-1} H^T \gamma \\
\text{s.t.} & \quad 0 \leq \gamma \leq c_2 e_1
\end{align*}
\]
(5)
where \(H = [A \quad e_1]\), \(G = [B \quad e_2]\), and \(\alpha\) and \(\gamma\) are the Lagrange multipliers.

The two hyperplanes can be obtained by solving the dual problems as follows:
\[
\begin{align*}
v_1 &= -(H^T H)^{-1} G^T \alpha, \quad v_1 = [w_1^T \quad b_1]^T, \\
v_2 &= -(G^T G)^{-1} H^T \gamma, \quad v_2 = [w_2^T \quad b_2]^T.
\end{align*}
\]
(6)
(7)

2.2 MLTSVM

For the multi-label problem, we denote the training set as:
\[
T = \{ (x_i, y_i) \}_{i=1, \ldots, m},
\]
(8)
where \(x_i \in \mathbb{R}^n\) is the training sample, \(y_i = \{y_{i1}, \ldots, y_{ip}\}\) is the label set of the sample \(x_i\), \(y_{iq} \in \{1, \ldots, K\}\) \((q = 1, \ldots, p)\), \(m\) is the total number of training samples and \(K\) is the total number of labels.

The MLTSVM seeks \(K\) hyperplanes:
\[
f_k(x) : w_k^T x + b_k = 0, \quad k = 1, 2, \ldots, K.
\]
(9)

We denote the samples belonging to the \(k\)th class by \(A_k\) and the other samples by \(B_k\). The original problem for label \(k\) is:
\[
\begin{align*}
\min_{w_k, b_k, \xi_k} & \quad \frac{1}{2} \|Aw_k + e_{A_k}b_k\|^2 + c_k \xi_k^T \xi_k + \frac{1}{2} \lambda_k (\|w_k\|^2 + b_k^2) \\
\text{s.t.} & \quad -(B_kw_k + e_{B_k}b_k) + \xi_k \geq e_{B_k}, \xi_k \geq 0
\end{align*}
\]
(10)
where \(c_k\) and \(\lambda_k\) are the penalty parameters, \(e_{A_k}\) and \(e_{B_k}\) are all 1 vector of the proper dimension, and \(\xi_{B_k}\) is the slack variable.
By introducing the Lagrange multiplier, the dual problems of (10) can be obtained as follows:

$$
\max_{x_{Bk}} \ e_{Bk}^T x_{Bk} - \frac{1}{2} x_{Bk}^T G (H^T H + \lambda_k I_k)^{-1} G^T x_{Bk},
$$

s.t. \ 0 \leq x_{Bk} \leq c_k

where $H = [A_k \ e_{A_k}]$, $G = [B_k \ e_{B_k}]$, $I_k$ are the diagonal matrices of the proper dimension, and $x_{Bk}$ is the Lagrange multiplier.

By solving the dual problem (11), we can obtain:

$$
u_k = -(H^T H + \lambda_k I_k)^{-1} G^T x_{Bk}, \ u_k = \left[ w_k^T \ b_k^T \right]^T.
$$

### 2.3 ML-STSVM

Similar to the MLTSVM, the ML-STSVM also seeks $K$ hyperplanes:

$$f_k(x) : w_k^T x + b_k = 0, \ k = 1, 2, \ldots, K.
$$

The original problem for label $k$ is:

$$
\min_{w_k, b_k, \xi_k} \frac{1}{2} \|A_k w_k + e_{A_k} b_k\|^2 + c_{k1} e_{B_k}^T \xi_k + \frac{1}{2} c_{k2}(\|w_k\|^2 + b_k^2) + \frac{1}{2} c_{k3}(w_k^T \Sigma_{A_k} w_k),
$$

s.t. \ -(B_k w_k + e_{B_k} b_k) + \xi_k \geq e_{B_k}, \ \xi_k \geq 0

where $c_{k3}(i = 1, 2, 3)$ are the penalty parameters, $\xi_k$ is the slack factor, $e_{A_k}$ and $e_{B_k}$ are all 1 vector of the proper dimension, and $\Sigma_{A_k} = \Sigma_1 + \ldots + \Sigma_i + \ldots + \Sigma_n$, $\Sigma_i$ is the covariance matrix of the $i$th cluster in $A_k$.

The dual problem of (14) is:

$$
\max_{x_{Bk}} \ e_{Bk}^T x_{Bk} - \frac{1}{2} x_{Bk}^T G (H^T H + c_{k2} I_k + c_{k3} J)^{-1} G^T x_{Bk},
$$

s.t. \ 0 \leq x_{Bk} \leq c_{k1}

where $H = [A_k \ e_{A_k}]$, $G = [B_k \ e_{B_k}]$, and $J = \left[ \Sigma_{A_k} 0 \right]$. $I_k$ are the diagonal matrices of the proper dimension, and $x_{Bk}$ is the Lagrange multiplier.

By solving the dual problem (15), we can obtain:

$$
u_k = -(H^T H + c_{k2} I_k + c_{k3} J)^{-1} G^T x_{Bk}, \ u_k = \left[ w_k^T \ b_k^T \right]^T.
$$

### 3 SS-MLTSVM

For the semi-supervised multi-label problem, we define the training set as follows:

$$T = \{ (x_i, y_i) | i = 1, \ldots, l \},
$$

where $x_i \in R^n$ is the training sample and $y_i = \{ y_{i1}, \ldots, y_{iK} \}$ is the label matrix of the sample $x_i$.

$$y_{ip} = \begin{cases} 
+1, & \text{if } x_i \text{ belongs to the } k \text{th class,} \\
-1, & \text{if } x_i \text{ doesn't belong to the } k \text{th class,} \\
0, & \text{uncertain,} \\
\end{cases} \quad 1 \leq p \leq K.
$$

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3.1 Manifold Regularization Framework

The manifold regularization framework [32], proposed by Belkin et al., can effectively solve semi-supervised learning problems. The objective optimization function of the manifold regularization framework can be expressed as follows:

$$f^* = \arg \min_{f \in \mathcal{H}} \sum_{i=1}^{l} V(x_i, y_i, f) + \gamma_H \|f\|^2_H + \gamma_M \|f\|^2_M,$$

(19)

where $f$ is the decision function to be solved, $V$ is the loss function on the labelled samples, the regularization term $\|f\|^2_H$ is used to control the complexity of the classifier, and the manifold regularization term $\|f\|^2_M$ reflects the internal manifold structure of the data distribution.

3.2 Linear SS-MLTSVM

Similar to the MLTSVM, for each label, the SS-MLTSVM seeks a hyperplane:

$$f_k(x) : w_k^T x + b_k = 0, \quad k = 1, 2, \ldots, K.$$

(20)

For the $k$th label, we denote the samples that definitely belong to the $k$th class by $A_k$, i.e., $A_k = \{x_i | y_i = +1\}$; the samples that definitely do not belong to the $k$th class by, i.e., $B_k = \{x_i | y_i = -1\}$; and the samples that are uncertain of belonging to the $k$th class, by $U_k$, i.e., $U_k = \{x_i | y_i = 0\}$; $T = A_k \cup B_k \cup U_k$.

To make full use of $U_k$, according to the manifold regularization framework, in our SS-MLTSVM, the loss function $V$ is replaced by a square loss function and a Hinge loss function, namely:

$$V(x_i, y_i, f_k) = ((A_i, w_k) + b_k)^2 + \max(0, 1 - f_k(B_i,))$$

(21)

The regularization term $\|f\|^2_H$ can be replaced by:

$$\|f_k\|^2_H = \frac{1}{2} (\|w_k\|^2 + b_k^2).$$

(22)

The manifold regularization term $\|f\|^2_M$ can be expressed as:

$$\|f_k\|^2_M = \frac{1}{2} \sum_{i,j=1}^{l} W_{ij} (f_k(x_i) - f_k(x_j))^2 = f_k^T L f_k,$$

(23)

where $f_k = [f_k(x_1), \ldots, f_k(x_l)]^T = Tw_k + eb_k$. $L = D - W$ is the Laplace matrix, where $W$ is defined as follows:

$$W_{ij} = \begin{cases} \exp(-\|x_i - x_j\|^2/2\sigma^2), & \text{if } x_i \text{ and } x_j \text{ are k nearest neighbor,} \\ 0, & \text{otherwise}, \end{cases}$$

(24)

and $D$ is defined as follows:

$$D_{ii} = \sum_{j=1}^{l_u} W_{ij}.$$
For the $k$th label, the original problem in the linear SS-MLTSVM is:

$$\begin{align*}
\min & \quad \frac{1}{2} (A_kw_k + e_Ab_k)^2 + c_k1 e_{B_k}^T \xi_{B_k} + \frac{1}{2} c_k2 \left( \|w_k\|^2 + b_k^2 \right) + \frac{1}{2} c_k3 (T w_k + e b_k)^T L(T w_k + e b_k) \\
\text{s.t.} & \quad - (B_kw_k + e_{B_k}b_k) + \xi_{B_k} \geq e_{B_k}, \quad \xi_{B_k} \geq 0
\end{align*}$$

(26)

where $c_{ki}(i = 1, 2, 3)$ are the penalty parameters, $\xi_{B_k}$ is the slack factor, $e_A$, $e_{B_k}$ and $e$ are all 1 vector of the proper dimension, and $L$ is the Laplace matrix.

The Lagrange function of (26) is as follows:

$$L(\Theta) = \frac{1}{2} (A_kw_k + e_Ab_k)^2 + c_k1 e_{B_k}^T \xi_{B_k} + \frac{1}{2} c_k2 \left( \|w_k\|^2 + b_k^2 \right) + \frac{1}{2} c_k3 (T w_k + e b_k)^T L(T w_k + e b_k) - x_{B_k}^T (-(B_kw_k + e_{B_k}b_k) + \xi_{B_k} - e_{B_k}) - \beta_{B_k}^T \xi_{B_k}$$

(27)

where $\Theta = \{ w_k, b_k, \xi_k, \alpha_{B_k}, \beta_{B_k} \}$. $\alpha_{B_k} \geq 0$ and $\beta_{B_k} \geq 0$ are Lagrange multipliers. Using KKT theory, we can obtain:

$$\frac{\partial L}{\partial w_k} = A_k^T (A_kw_k + e_Ab_k) + c_k2 w_k + c_k3 T^T L(T w_k + e b_k) + B_k^T \alpha_{B_k} = 0,$$

(28)

$$\frac{\partial L}{\partial b_k} = e_{A_k}^T (A_kw_k + e_Ab_k) + c_k2 b_k + c_k3 e^T L(T w_k + e b_k) + e_{B_k}^T \alpha_{B_k} = 0,$$

(29)

$$\frac{\partial L}{\partial \xi_k} = c_k1 e_{B_k} - \alpha_{B_k} - \beta_{B_k} = 0.$$

(30)

According to (28)–(30), we can obtain the dual problem of (26) as follows:

$$\max_x e_{B_k}^T \alpha_{B_k} - \frac{1}{2} x_{B_k}^T G (H^T H + c_k2 I_k + c_k3 J^T L J)^{-1} G^T \alpha_{B_k},$$

s.t. $0 \leq \alpha_{B_k} \leq c_k1 e_{B_k}$

(31)

where $H = [A_k \quad e_{A_k}]$, $G = [B_k \quad e_{B_k}]$, and $J = [T \quad e]$.

For the $k$th label, the hyperplane can be obtained by solving the dual problem as follows:

$$v_k = - (H^T H + c_k2 I_k + c_k3 J^T L J)^{-1} G^T \alpha_{B_k}, \quad v_k = [w_k^T \quad b_k^T]^T.$$  

(32)

### 3.3 Nonlinear SS-MLTSVM

In this section, using the kernel-generated surfaces, we extend the linear SS-MLTSVM to the nonlinear case. For each label, the nonlinear SS-MLTSVM seeks the following hyperplanes:

$$f_k(x) : K(x^T, T^T)w_k + b_k = 0, \quad k = 1, 2, \ldots, K,$$

(33)

where $K(\cdot, \cdot)$ is a kernel function. Similar to the linear case, the regularization term $\|f_k\|^2_H$ and the manifold regularization term $\|f_k\|^2_M$ in (19) can be, respectively, expressed as:

$$\|f_k\|^2_H = \frac{1}{2} (w_k^T K(T, T^T) w_k + b_k^2);$$

(34)

$$\|f_k\|^2_M = f_k^T L f_k = (K(T, T^T) w_k + e b_k)^T L (K(T, T^T) w_k + e b_k).$$

(35)
The original problem of the nonlinear SS-MLTSVM is as follows:
\[
\min \frac{1}{2} (K(A_k, T^T)w_k + e_{A_k}b_k)^2 + \frac{1}{2}c_{k1}e_{B_k}^T \xi B_k + \frac{1}{2}c_{k2}(w_k^T K(T, T^T)w_k + b_k^2) \\
+ \frac{1}{2}c_{k3}(K(T, T^T)w_k + eb_k)^T L(K(T, T^T)w_k + eb_k) \\
s.t. - (K(B_k, T^T)w_k + e_{B_k}b_k) + \xi B_k \geq e_{B_k}, \xi B_k \geq 0
\]
\[\text{(36)}\]

The Lagrange function of (36) is as follows:
\[
L(\Theta) = \frac{1}{2} (K(A_k, T^T)w_k + e_{A_k}b_k)^2 + \frac{1}{2}c_{k1}e_{B_k}^T \xi B_k + \frac{1}{2}c_{k2}(w_k^T K(T, T^T)w_k + b_k^2) \\
+ \frac{1}{2}c_{k3}(K(T, T^T)w_k + eb_k)^T L(K(T, T^T)w_k + eb_k) \\
- 2\xi B_k \left( - (K(B_k, T^T)w_k + e_{B_k}b_k) + \xi B_k - e_{B_k} \right) - \beta B_k \xi B_k
\]
\[\text{(37)}\]

According to KKT theory, we can obtain:
\[
\frac{\partial L}{\partial w_k} = K(A_k, T^T)^T (K(A_k, T^T)w_k + e_{A_k}b_k) + c_{k2}K(T, T^T)w_k \\
+ c_{k3}K(T, T^T) L(K(T, T^T)w_k + eb_k) + K(B_k, T^T) b_k = 0
\]
\[\text{(38)}\]
\[
\frac{\partial L}{\partial b_k} = e_{A_k}^T (K(A_k, T^T)w_k + e_{A_k}b_k) + c_{k2}b_k + c_{k3}e^T L(K(T, T^T)w_k + eb_k) + e_{B_k} b_k = 0,
\]
\[\text{(39)}\]
\[
\frac{\partial L}{\partial \xi k} = c_{k1}e_{B_k} - \xi B_k - \beta B_k = 0.
\]
\[\text{(40)}\]

According to (38)–(40), we can obtain the dual problem of (32) as follows:
\[
\max \sum x e_{B_k}^T \xi B_k - \frac{1}{2} \xi B_k G (H^T H + c_{k2} I_k + c_{k3} J^T L J)^{-1} G^T \xi B_k,
\]
\[\text{s.t. } 0 \leq \xi B_k \leq c_{k1} e_{B_k}
\]
\[\text{where } H = [ K(A_k, T^T) e_{A_k} ], G = [ K(B_k, T^T) e_{B_k} ], J = [ K(T, T^T) e ] \text{ and } I_k = \begin{bmatrix} K(T, T^T) & 0 \\ 0 & 1 \end{bmatrix}.
\]

By solving the dual problem, the hyperplane of the \(k\)th label can be obtained as follows:
\[
v_k = -(H^T H + c_{k2} I_k + c_{k3} J^T L J)^{-1} G^T \xi B_k, \quad v_k = \begin{bmatrix} w_k^T \\ b_k^T \end{bmatrix}^T.
\]
\[\text{(42)}\]

3.4 Decision Function

In this subsection, we present the decision function of our SS-MLTSVM. For a new sample \(x\), as mentioned above, if the sample \(x\) is proximal enough to a hyperplane, it can be assigned to the corresponding class. In other words, if the distance \(d_k(x)\) between \(x\) and the \(k\)th hyperplane
\[
d_k(x) = \frac{|w_k^T x + b_k|}{||w_k||}, \quad k = 1, \ldots, K,
\]
\[\text{(43)}\]
is less than or equal to the given value $\Delta_k$, $k = 1, \ldots, K$, then the sample $x$ is assigned to the $k$th class. To choose the proper $\Delta_k$, we apply the strategy in the MLTSVM, which is a simple and effective method, i.e., we set $\Delta_k = \Delta = \min_{p=1,\ldots,K} \left( \frac{1}{\|w_p\|^2} \right)$, $k = 1, \ldots, K$.

### 3.5 Fast Solvers

In this subsection, we use SOR to solve the dual problems (31) and (41) efficiently [33]. For convenience, we set $Q = G(H^TH + c_{k2}I_k + c_{k3}J^TLJ)^{-1}G^T$. The dual problems (31) and (41) can be uniformly rewritten as:

$$\begin{align*}
\max_{x} & \quad e^T_k x_k - \frac{1}{2} x_k^T Q x_k, \\
\text{s.t.} & \quad 0 \leq x_k \leq c_{k1} e_{B_k},
\end{align*}$$

(44)

Algorithm 1: The SOR for optimization problem (44)

INPUT:

- penalty parameter $c_{k1}$, relaxation factor $t \in (0, 2)$, and matrix $Q$.

OUTPUT:

The optimal solution $x_k$ in (44).

Step 1: Initialize the iteration variable $i = 0$ and start with any $x^0$.

Step 2: Decompose $Q = S + M + S'$, where $M$ is a diagonal matrix and $S$ is a strict lower triangular matrix.

Step 3: While $\|x^{i+1} - x^i\| < \sigma$

- Calculate $x^{i+1} = x^i + t \Delta x$, where $\Delta x = -M^{-1}(Qx^i - e + S'(x^{i+1} - x^i))$.
- Project $x^{i+1} \in [0, c_{k1}]$.

End while.

Algorithm 1 only updates one variable $x^{i+1}$ in each iteration, which can effectively reduce the complexity of the algorithm and speed up the learning process.

### 4 Experiments

In this section, we present the classification results of backpropagation for multi-label learning (BPMLL) [34], ML-kNN, Rank-SVM, MLTSVM and our SS-MLTSVM on the benchmark datasets. All the algorithms are implemented in MATLAB (R2017b), and the experimental environment is an Intel Core i3 processor and 4G RAM. In the experiments, we use five common datasets for multi-label learning, including flags, birds, emotions, yeast and scene (see Tab. 1). To verify the classification performance of our SS-MLTSVM, we choose 50% of the dataset as labelled samples and the remaining samples as unlabelled samples.

The parameters of the algorithm have an important impact on the classification performance. We use 10-fold cross-validation to select the appropriate parameters for each algorithm. For BPMLL, the number of hidden neurons is set to 20% of the input dimension, and the number of training epochs is 100. For the ML-kNN, the number of nearest neighbours is set to 5. For the Rank-SVM, the penalty parameter $c$ is
selected from $\{2^{-8}, \ldots, 2^0, \ldots, 2^8\}$. For the MLTSVM, we select penalty parameters $c_k$ and $\lambda_k$ from $\{2^{-8}, \ldots, 2^0, \ldots, 2^8\}$. For the SS-MLTSVM, we select penalty parameters $c_{k1}$, $c_{k2}$, and $c_{k3}$ from $\{2^{-8}, \ldots, 2^0, \ldots, 2^8\}$.

Table 1: Detailed description of the datasets

| Datasets | Domain | Unlabelled Instance | Labelled Instance | Feature | Label |
|----------|--------|---------------------|-------------------|---------|-------|
| Flags    | image  | 97                  | 97                | 19      | 7     |
| Birds    | audio  | 322                 | 323               | 260     | 19    |
| Emotions | music  | 296                 | 297               | 72      | 6     |
| Scene    | image  | 1203                | 1204              | 294     | 6     |
| Yeast    | biology| 1235                | 1236              | 103     | 14    |

4.1 Evaluation Criteria

In the experiments, we use five popular metrics to evaluate the multi-label classifiers, which are Hamming loss, average precision, coverage, one_error and ranking loss. Next, we introduce these five evaluation metrics in detail.

We denote the total number of samples by $l$ and the total number of labels by $K$. $Y_i$ and $\overline{Y}_i$ represent the relevant label set and irrelevant label set of sample $x_i$, respectively. The function $f(x,y)$ returns a confidence of $y$ being the right label of sample $x$, and the function $rank(x,y,f)$ returns a descending rank of $f(x,y)$ for any $y \in \{y_1, \ldots, y_K\}$.

4.1.1 Hamming Loss

The evaluation criteria are used to measure the proportion of labels that are wrongly classified.

$$\text{Hamming Loss}(H_L) = \frac{1}{l} \sum_{i=1}^{l} \frac{1}{K} |h(x_i) \Delta Y_i|, \quad (45)$$

where $h(x_i)$ is the predicted label set of sample $x_i$.

4.1.2 Coverage

The evaluation criteria are used to measure how many steps we need to go down the ranked label list to contain all true labels of a sample.

$$\text{Coverage} = \frac{1}{l} \sum_{i=1}^{l} \max_{y \in Y_i} \text{rank}(x_i,y,f) - 1. \quad (46)$$

4.1.3 One_Error

The evaluation criteria are used to measure the proportion of samples whose label with the highest prediction probability is not in the true label set.
\[ One \_ error(O,E) = \frac{1}{l} \sum_{i=1}^{l} H(x_i), \]  

where

\[ H(x_i) = \begin{cases} 0 & \text{if } \arg \max f(x_i, y) \in Y_i, \\ 1 & \text{otherwise} \end{cases} \]  

4.1.4 Ranking Loss

The evaluation criteria are used to measure the proportion of label pairs that are ordered reversely.

\[ Ranking \_ loss(R_L) = \frac{1}{l} \sum_{i=1}^{l} \left( \frac{1}{|Y_i|} \sum_{|y' \subseteq Y_i|} \left| \left\{ y'y'' \mid f(x_i,y') \leq f(x_i,y''), \ y' \in Y_i, \ y'' \in \overline{Y_i} \right\} \right| \right) \]  

4.1.5 Average Precision

The evaluation criteria are used to measure the proportion of labels ranked above a particular label \( y \in Y_i \).

\[ Average \_ precision(A_P) = \frac{1}{l} \sum_{i=1}^{l} \left( \frac{1}{|Y_i|} \sum_{y \in Y_i} \left| \left\{ (y' \in Y_i) \mid rank(x_i,y',f) \leq rank(x_i,y,f) \right\} \right| \right) \]  

4.2 Results

We show the average precision, coverage, Hamming loss, one_error and ranking loss of each algorithm on the benchmark datasets in Tabs. 2–6. From Tabs. 2 and 3, we can observe that, for average precision and coverage, our SS-MLTSVM is superior to the other algorithms for each dataset, while for Hamming loss, one_error and ranking loss, no algorithm is superior to any other algorithm on all datasets. Therefore, for Hamming loss, one_error and ranking loss, we proceed to use the Friedman test to evaluate each algorithm statistically. The Friedman statistics is as follows:

\[ \chi^2_F = \frac{12N}{k(k+1)} \sum_{j} R_j^2 - \frac{k(k+1)^2}{4} \]  

where \( R_j = \frac{1}{N} \sum r_j' \), \( r_j' \) represents the rank of the \( j \)th algorithm on the \( i \)th dataset. Because \( \chi^2_F \) is undesirably conservative, we apply the better statistic

\[ F_F = \frac{(N-1)\chi^2_F}{N(k-1)-\chi^2_F} \sim F(k-1,(k-1)(N-1)) \]  

where \( k \) is the number of algorithms and \( N \) is the number of datasets.

We can obtain \( \chi^2_F(H,L) = 7.84 \), \( \chi^2_F(O,E) = 9.76 \), \( \chi^2_F(R,L) = 9.92 \), and \( F_F(H,L) = 2.58 \), \( F_F(O,E) = 3.81 \), \( F_F(R,L) = 3.94 \). When the significance level is \( \alpha = 0.10 \), \( F(4,16) = 2.33 \). Because \( F_F(H,L) = 2.58 \), \( F_F(O,E) = 3.81 \) and \( F_F(R,L) = 3.94 \) are larger than the critical values, 5 algorithms have significant differences for the three metrics. We list the rank of the different algorithms in light of Hamming loss, one_error and ranking loss in Tabs. 7–9. From Tabs. 7–9, we can see that the average rank of our SS-MLTSVM is better than other algorithms; thus, the SS-MLTSVM has better classification performance.
| Table 2: Average precision of algorithms on the benchmark datasets |
|---------------------------------------------|
| BPMLL | ML-kNN | Rank-SVM | MLTSVM | SS-MLTSVM |
| Flags | 0.785639 ± 0.051239 | 0.793221 ± 0.008711 | 0.795623 ± 0.003876 | 0.777998 ± 0.009513 | **0.800176 ± 0.008125** |
| Birds | 0.358771 ± 0.010801 | 0.421682 ± 0.008798 | 0.406008 ± 0.003114 | 0.404525 ± 0.005299 | **0.449760 ± 0.004186** |
| Emotions | 0.581655 ± 0.030349 | 0.697028 ± 0.004776 | 0.709426 ± 0.005503 | 0.757375 ± 0.005520 | **0.811084 ± 0.006444** |
| Scene | 0.453430 ± 0.020162 | 0.842465 ± 0.003841 | 0.830496 ± 0.002475 | 0.827238 ± 0.002951 | **0.845295 ± 0.004920** |
| Yeast | 0.720021 ± 0.023814 | 0.731047 ± 0.000957 | 0.730825 ± 0.000957 | 0.731715 ± 0.000454 | **0.744821 ± 0.001117** |

| Table 3: Coverage of algorithms on the benchmark datasets |
|---------------------------------------------|
| BPMLL | ML-kNN | Rank-SVM | MLTSVM | SS-MLTSVM |
| Flags | 3.875556 ± 0.663135 | 3.777000 ± 0.031977 | 3.797440 ± 0.024735 | 3.837778 ± 0.082848 | **3.771110 ± 0.054257** |
| Birds | 3.923201 ± 0.073242 | 4.101629 ± 0.052476 | 3.889508 ± 0.029002 | 3.482169 ± 0.028734 | **3.133523 ± 0.063058** |
| Emotions | 2.868046 ± 0.294812 | 2.245276 ± 0.034788 | 2.191575 ± 0.032059 | 2.044092 ± 0.035888 | **1.842989 ± 0.057524** |
| Scene | 2.171729 ± 0.141061 | 0.555427 ± 0.008191 | 0.598790 ± 0.007469 | 0.612847 ± 0.011171 | **0.523698 ± 0.014979** |
| Yeast | 6.341873 ± 0.342050 | 6.456955 ± 0.022583 | 6.231757 ± 0.010173 | 6.987227 ± 0.024749 | **6.222335 ± 0.042419** |

| Table 4: Hamming loss of algorithms on the benchmark datasets |
|---------------------------------------------|
| BPMLL | ML-kNN | Rank-SVM | MLTSVM | SS-MLTSVM |
| Flags | 0.347143 ± 0.028855 | 0.329460 ± 0.009443 | 0.306206 ± 0.006918 | 0.315238 ± 0.009461 | **0.301361 ± 0.012386** |
| Birds | 0.067793 ± 0.001566 | **0.055723 ± 0.000044** | 0.106989 ± 0.003470 | 0.097220 ± 0.001389 | 0.087929 ± 0.001621 |
| Emotions | 0.374502 ± 0.040605 | 0.263362 ± 0.003004 | 0.264391 ± 0.003745 | 0.229292 ± 0.003495 | **0.206513 ± 0.007170** |
| Scene | 0.285943 ± 0.019638 | 0.151188 ± 0.003112 | **0.090790 ± 0.000977** | 0.184711 ± 0.00128 | 0.147302 ± 0.001591 |
| Yeast | 0.216659 ± 0.016479 | 0.212532 ± 0.000808 | 0.212260 ± 0.001056 | 0.210753 ± 0.001176 | **0.209740 ± 0.001138** |

| Table 5: One_error of algorithms on the benchmark datasets |
|---------------------------------------------|
| BPMLL | ML-kNN | Rank-SVM | MLTSVM | SS-MLTSVM |
| Flags | 0.262222 ± 0.012525 | 0.246806 ± 0.029941 | 0.195583 ± 0.021652 | 0.238889 ± 0.022773 | **0.161905 ± 0.023462** |
| Birds | 0.765142 ± 0.019694 | **0.633331 ± 0.012700** | 0.642681 ± 0.004973 | 0.733791 ± 0.012932 | 0.686058 ± 0.012041 |
| Emotions | 0.634943 ± 0.051561 | 0.412047 ± 0.014014 | 0.383724 ± 0.012444 | 0.296793 ± 0.006964 | **0.232759 ± 0.007655** |
| Scene | 0.820441 ± 0.026645 | 0.269452 ± 0.003841 | 0.278494 ± 0.004690 | 0.287614 ± 0.004593 | **0.252672 ± 0.009250** |
| Yeast | 0.240158 ± 0.036489 | 0.265893 ± 0.003882 | 0.241793 ± 0.002361 | 0.249052 ± 0.003871 | **0.232493 ± 0.003846** |

| Table 6: Ranking loss of algorithms on the benchmark datasets |
|---------------------------------------------|
| BPMLL | ML-kNN | Rank-SVM | MLTSVM | SS-MLTSVM |
| Flags | 0.229981 ± 0.043959 | 0.228139 ± 0.008245 | **0.216063 ± 0.00325** | 0.239685 ± 0.010365 | 0.229881 ± 0.009013 |
| Birds | 0.313953 ± 0.006586 | 0.318532 ± 0.004400 | 0.302169 ± 0.004040 | 0.292203 ± 0.002815 | **0.250932 ± 0.004507** |
| Emotions | 0.392612 ± 0.039955 | 0.266880 ± 0.004724 | 0.253129 ± 0.005824 | 0.216821 ± 0.006205 | **0.169383 ± 0.008775** |
| Scene | 0.418993 ± 0.028879 | 0.098806 ± 0.001565 | 0.105142 ± 0.001448 | 0.124898 ± 0.002293 | **0.085024 ± 0.002948** |
| Yeast | 0.185699 ± 0.001101 | 0.181432 ± 0.000784 | **0.171814 ± 0.000470** | 0.217908 ± 0.000920 | 0.174228 ± 0.021022 |
From the above analysis, we can conclude that our SS-MLTSVM is superior to the other algorithms for all metrics.

We show the learning time of different algorithms on the benchmark datasets in Tab. 10. From Tab. 10, we can observe that our SS-MLTSVM has a lower learning speed than the MLTSVM. This is mainly because our SS-MLTSVM adds a manifold regularization term that needs to solve the Laplace matrix with whole samples. Even so, our SS-MLTSVM still has great advantages compared with the Rank-SVM and BPMLL.

### Table 7: Ranks of algorithms in light of Hamming loss

|          | BPMLL | ML-kNN | Rank-SVM | MLTSVM | SS-MLTSVM |
|----------|-------|--------|----------|--------|-----------|
| Flags    | 5     | 4      | 2        | 3      | 1         |
| Birds    | 2     | 1      | 5        | 4      | 3         |
| Emotions | 5     | 3      | 4        | 2      | 1         |
| Scene    | 5     | 3      | 1        | 4      | 2         |
| Yeast    | 5     | 4      | 3        | 2      | 1         |
| Average  | 4.4   | 3      | 3        | 3      | 1.6       |

### Table 8: Ranks of algorithms in light of one_error

|          | BPMLL | ML-kNN | Rank-SVM | MLTSVM | SS-MLTSVM |
|----------|-------|--------|----------|--------|-----------|
| Flags    | 5     | 4      | 2        | 3      | 1         |
| Birds    | 5     | 1      | 2        | 4      | 3         |
| Emotions | 5     | 4      | 3        | 2      | 1         |
| Scene    | 5     | 2      | 3        | 4      | 1         |
| Yeast    | 2     | 5      | 3        | 4      | 1         |
| Average  | 4.4   | 3.2    | 2.6      | 3.4    | 1.4       |

### Table 9: Ranks of algorithms in light of ranking loss

|          | BPMLL | ML-kNN | Rank-SVM | MLTSVM | SS-MLTSVM |
|----------|-------|--------|----------|--------|-----------|
| Flags    | 4     | 2      | 1        | 5      | 3         |
| Birds    | 4     | 5      | 3        | 2      | 1         |
| Emotions | 5     | 4      | 3        | 2      | 1         |
| Scene    | 5     | 2      | 3        | 4      | 1         |
| Yeast    | 4     | 3      | 1        | 5      | 2         |
| Average  | 4.4   | 3.2    | 2.2      | 3.6    | 1.6       |
4.3 Sensitivity Analysis

In this subsection, we investigate the effect of the size of unlabelled samples on the classification performance. In Figs. 1–5, we show the classification performance of our SS-MLTSVM and the MLTSVM on different datasets for different sizes of unlabelled samples.

From Figs. 1–5, we can observe that the classification performance of the SS-MLTSVM is better than that of the MLTSVM in all cases. With the increase of unlabelled samples, the advantages of the SS-MLTSVM become increasingly obvious, because, with the increase of in unlabelled samples, the SS-MLTSVM can make full use of the embedded geometric information, construct a more reasonable classifier, and further improve the classification performance.

| Table 10: Learning time of algorithms on the benchmark datasets |
|-------------------|-------------------|-------------------|-------------------|-------------------|
|                   | BPMLL             | ML-kNN            | Rank-SVM          | MLTSVM            | SS-MLTSVM         |
| Flags             | 4.808817          | 0.050400          | 0.359997          | **0.050300**      | 0.074584          |
| Birds             | 16.868832         | **0.139376**      | 4.273635          | 0.187632          | 1.566527          |
| Emotions          | 17.929608         | **0.147162**      | 1.282045          | 0.384163          | 1.153655          |
| Scene             | 154.982600        | **1.913366**      | 5.794408          | 4.145783          | 12.102076         |
| Yeast             | 69.403602         | **2.093822**      | 49.447880         | 19.581926         | 38.792532         |
| Average           | 52.798700         | 0.868840          | 12.231600         | **4.869937**      | 10.737873         |

Figure 1: Average precision of the SS-MLTSVM and MLTSVM for unlabelled samples of different sizes

Figure 2: Hamming loss of the SS-MLTSVM and MLTSVM for unlabelled samples of different sizes
In this paper, a novel SS-MLTSVM is proposed to solve semi-supervised multi-label classification problems. By introducing the manifold regularization term into the MLTSVM, we construct a more reasonable classifier and use SOR to speed up learning. Theoretical analysis and experimental results show that, compared with the existing multi-label classifiers, the SS-MLTSVM can take full advantage of
the geometric information embedded in partially labelled and unlabelled samples and effectively solve semi-supervised multi-label classification problems. It should be pointed out that our SS-MLTSVM does not consider the correlation among labels; however, the correlation among labels is very valuable to improve the generalization performance. Therefore, more effective methods of obtaining correlation among labels should be addressed in the future.

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