Vietnam Journal of Computer Science

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--Manuscript Draft--

Manuscript Number:	WSPC-VJCS-D-24-00193
Full Title:	Twin Support Vector Machine with Multi-Clusters Data
Article Type:	Research Paper
Keywords:	Support Vector Machine; Twin Support Vector Machine; Structural Twin Support Vector Machine; Structural granularity.
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Twin Support Vector Machine with Multi-Clusters Data

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Received (Day Month Year)
Revised (Day Month Year)

With the rapid development of data, data sets are increasing in number and diversifying in structure. In binary classification problems, two data classes seem to be more complicated due to the number of data points of clusters in each class being different. Traditional algorithms such as Support Vector Machines (SVM) don't sufficiently exploit data information: structural information with cluster granularity and information about the number of data points in each cluster. This may affect the accuracy of binary classification problems. This paper proposes a new method to deal with binary classification problems for multi-clusters data, a Twin Support Vector Machine with Multi-Clusters Data (called TSVM-MCD) using a cluster-vs-class strategy. Both theoretically and experimentally, we show the comparison of TSVM-MCD with two improvements of SVM.

Keywords: Support Vector Machine, Twin Support Vector Machine, Structural Twin Support Vector Machine, Structural granularity.

1. Introduction

In the latter half of the 20th century, the issue of classifying data into two categories was first introduced and explored. However, the data sets collected during that time were relatively simple. As time passed, real-world data became more diverse in structure and quantity. Different clusters often establish data sets, each cluster has one distributed trend and the number of data points of each cluster is different (multi-clusters data). For example, we consider the problem of classifying fruits with data including five categories: Mango, Jackfruit, Pineapple, Apples, and Grapes, but the fruits will only be classified according to the criteria "smooth skin" or "rough skin". Data in the "smooth skin" class will form 3 clusters, corresponding

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to Mango, Apples, and Grapes. In comparison, data in the "rough skin" class will be distributed into 2 clusters, corresponding to Jackfruit and Pineapple.

As a result, binary classification algorithms also needed to be improved to better handle the increasing diversity of data. Support Vector Machine (SVM)[1,2] was a popular binary classification algorithm applied to many different fields in practice.[3–7] The main idea of SVM is to find a hyperplane separating two classes with the largest margin. However, SVM does not fully exploit structural information and information about the number of data points of clusters. Many variants of SVM have been recently proposed to improve the accuracy and other tasks of standard SVM.[6–10] Two typical innovations of SVM are the Twin Support Vector Machine (TSVM),[11] and the Structural Twin Support Vector Machine (S-TSVM).[12] The main idea of TSVM is to seek two hyperplanes such that each hyperplane is closer to one class and put the remaining class to one side by solving two Quadratic Programming Problems (QPPs)[13] whose sizes are smaller than the QPP in SVM. S-TSVM has the same strategy as TSVM. Besides, S-TSVM fully exploits structural information with cluster granularity into learning the model to build a more reasonable classifier. However, both TSVM and S-TSVM don't use information about the number of data points in each cluster.

Based on the strategy of TSVM[11] and S-TSVM,[12] we propose a new binary classification model: Twin Support Vector Machine with Multi-Clusters Data (called TSVM-MCD) with a cluster-vs-class strategy. Instead of solving two QPPs as in S-TSVM, TSVM-MCD will solve $(k + l)$ QPPs, where k and l are the number of clusters in class $\{+\}$ and class $\{-\}$, respectively. This method allows TSVM-MCD to effectively describe the distribution trend of each cluster in each class, so its ability to generalize data is better and may improve classification accuracy for binary classification problems with multi-clusters data.

The paper is organized as follows: Section 2 briefly introduces the background of QPP, Structural granularity, SVM, TSVM, and S-TSVM; Section 3 is a detailed description of TSVM-MCD along with the algorithms and discussions; All experimental results are shown in Section 4, together with the comparative evaluation; The conclusion is given in Section 5. All algorithms are settled by Python Programming Language.

In this paper, all real numbers are denoted by normal letters, all vectors will be column vectors and denoted by bold letters, transformed to a row vector by ^{T}. A column vector of ones in real space of arbitrary dimension will be denoted by $\mathbf{e}$. All matrices will be denoted by bold capital letters. The identity matrix of arbitrary dimension will be denoted by $\mathbf{I}$, and $\|\|$ is the Euclidean norm.

2. Background

In this section, we first briefly describe the background of QPP, Structural granularity, SVM,[1] TSVM,[11] and S-TSVM.[12]

2.1. *The Quadratic Programming Problem.*

The general form of the problem is as follows:

$$\text{QPP}: \begin{cases} Q(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T\mathbf{G}\mathbf{x} + \mathbf{g}^T\mathbf{x} + \alpha \longrightarrow \min, \\ \mathbf{p}_i^T\mathbf{x} \geq b_i, \quad i \in I := \{1, \ldots, p\}, \\ \mathbf{q}_j^T\mathbf{x} = d_j, \quad j \in J := \{1, \ldots, q\}. \end{cases}$$

By setting $\mathbf{P} = [\mathbf{p}_1, \ldots, \mathbf{p}_p]^T$ is the matrix consisting of p row vectors $\mathbf{p}_i^T$, $\mathbf{Q} = [\mathbf{q}_1, \ldots, \mathbf{q}_q]^T$ is the matrix consisting of q row vectors $\mathbf{q}_j^T$, $\mathbf{b} = (b_1, b_2, \ldots, b_p)$, $\mathbf{d} = (d_1, d_2, \ldots, d_q)$.

The matrix form of the QPP is as follows:

$$\text{QPP}: \begin{cases} Q(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T\mathbf{G}\mathbf{x} + \mathbf{g}^T\mathbf{x} + \alpha \longrightarrow \min, \\ \mathbf{P}\mathbf{x} \geq \mathbf{b}, \\ \mathbf{Q}\mathbf{x} = \mathbf{d}. \end{cases}$$

Where $\mathbf{G} \in \mathbb{R}^{n\times n}$ is the symmetric matrix, $\mathbf{P} \in \mathbb{R}^{p\times n}$, $\mathbf{Q} \in \mathbb{R}^{q\times n}$, $\mathbf{b} \in \mathbb{R}^p$, $\mathbf{d} \in \mathbb{R}^q$, $\mathbf{g}, \mathbf{x} \in \mathbb{R}^n$, $\alpha \in \mathbb{R}$. When the objective function Q is convex (i.e. $\mathbf{G}$ is positive semi-definite), the QPP is a convex problem.

Theorem 2.1 (Optimal conditions (see Ref. 13, pp. 412)).

(a) Suppose that $\mathbf{x}^*$ is the solution of QPP. Then there are coefficients $\boldsymbol{\lambda}^* = (\lambda_1^*, \ldots, \lambda_p^*) \in \mathbb{R}^p$, $\boldsymbol{\mu}^* = (\mu_1^*, \ldots, \mu_q^*) \in \mathbb{R}^q$ satisfying the following conditions:

$$\begin{cases} \mathbf{G}\mathbf{x}^* + \mathbf{g} = \sum_{i=1}^{p} \lambda_i^* \mathbf{p}_i + \sum_{j=1}^{q} \mu_j^* \mathbf{q}_j, & \\ \mathbf{p}_i^T\mathbf{x}^* \geq b_i,\ \lambda_i^* \geq 0, & i \in I = \{1, \ldots, p\}, \\ \lambda_i^*(\mathbf{p}_i^T\mathbf{x}^* - b_i) = 0, & i \in I, \\ \mathbf{q}_j^T\mathbf{x}^* = d_j, & j \in J = \{1, \ldots, q\}. \end{cases}$$

The above conditions are called the KKT system ($Karush - Kuhn - Tucker$) of QPP, $\mathbf{x}^*$ is called a KKT point, and the coefficients $\boldsymbol{\lambda}^*$, $\boldsymbol{\mu}^*$ are called Lagrange multipliers corresponding to $\mathbf{x}^*$.

(b) If the QPP is convex, and $\mathbf{x}^*$ is a KKT point with Lagrange multipliers $\boldsymbol{\lambda}^*$, $\boldsymbol{\mu}^*$, then $\mathbf{x}^*$ is also a solution of QPP.

Note that, the KKT system can be rewritten in the matrix form as follows:

$$\begin{cases} \mathbf{G}\mathbf{x}^* + \mathbf{g} = \mathbf{P}^T\boldsymbol{\lambda}^* + \mathbf{Q}^T\boldsymbol{\mu}^*, \\ \mathbf{P}\mathbf{x}^* \geq \mathbf{b},\ \boldsymbol{\lambda}^* \geq \mathbf{0}, \\ \boldsymbol{\lambda}^{*T}(\mathbf{P}\mathbf{x}^* - \mathbf{b}) = \mathbf{0}, \\ \mathbf{Q}\mathbf{x}^* = \mathbf{d}. \end{cases}$$

2.2. *Structural granularity*

Consider a binary classification problem with the multi-clusters data set, denoted by a matrix $\mathbf{C}$, consisting of m points (each point is a row of $\mathbf{C}$) $\mathbf{x}_j^T \in \mathbb{R}^n$, $1 \leq j \leq m$. We also write $\mathbf{x}_j \in \mathbf{C}$ to indicate that $\mathbf{x}_j$ is a row of $\mathbf{C}$. Suppose that $y_j \in \{-1, 1\}$ is the $j-$th data point label corresponding to $\mathbf{x}_j$. Class $\{+\}$ consists of m_A points denoted by a matrix $\mathbf{A} \subset \mathbb{R}^{m_A \times n}$, and class $\{-\}$ consists of m_B points denoted by a matrix $\mathbf{B} \subset \mathbb{R}^{m_B \times n}$. There are k clusters in class $\mathbf{A}$, whose $i-$th cluster consists of m_{Ai} points and is denoted by matrix $\mathbf{A}_i \subset \mathbb{R}^{m_{Ai} \times n}, i = 1, \ldots, k$. Also, there are l clusters in class $\mathbf{B}$, whose $j-$th cluster consists of m_{Bj} points and is denoted by matrix $\mathbf{B}_j \subset \mathbb{R}^{m_{Bj} \times n}, j = 1, \ldots, l$. Here, $\mathbf{A}$, $\mathbf{B}$, $\mathbf{A}_i$, $\mathbf{B}_j$ are called structural granularity.[14] We are interested in the following quantities of structural granularity.

- Class granularity:
  $\Sigma_A = \frac{1}{m_A} \sum\limits_{\mathbf{x}_j \in \mathbf{A}} (\mathbf{x}_j - \boldsymbol{\mu}_A)(\mathbf{x}_j - \boldsymbol{\mu}_A)^T$,
  $\Sigma_B = \frac{1}{m_B} \sum\limits_{\mathbf{x}_j \in \mathbf{B}} (\mathbf{x}_j - \boldsymbol{\mu}_B)(\mathbf{x}_j - \boldsymbol{\mu}_B)^T$.
- Cluster granularity:
  $\Sigma_{Ai} = \frac{1}{m_{Ai}} \sum\limits_{\mathbf{x}_j \in \mathbf{A}_i} (\mathbf{x}_j - \boldsymbol{\mu}_{Ai})(\mathbf{x}_j - \boldsymbol{\mu}_{Ai})^T$,
  $\Sigma_{Bj} = \frac{1}{m_{Bj}} \sum\limits_{\mathbf{x}_j \in \mathbf{B}_j} (\mathbf{x}_j - \boldsymbol{\mu}_{Bj})(\mathbf{x}_j - \boldsymbol{\mu}_{Bj})^T$.

Here, $\boldsymbol{\mu}_X$ denotes the average vector of the data set $\mathbf{X}$. When the data set is standardized we have $\Sigma_X = \frac{1}{m_X}\mathbf{X}^T\mathbf{X}$

2.3. *SVM, TSVM, S-TSVM*

The main idea of Support Vector Machines (SVM)[1] is to seek a hyperplane

$$f(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + b = 0, \quad \mathbf{w} \in \mathbb{R}^n, b \in \mathbb{R},$$

which separates class $\mathbf{A}$ and class $\mathbf{B}$ such that the margin $\frac{2}{\|\mathbf{w}\|}$ between the two classes is the largest, by solving the QPP as follows:

$$\begin{cases} \min\limits_{\mathbf{w},\ b,\ \boldsymbol{\xi}} & c\mathbf{e}^T\boldsymbol{\xi} + \frac{1}{2}\|\mathbf{w}\|^2, \\ \text{s.t.} & \mathbf{D}(\mathbf{C}\mathbf{w} + \mathbf{e}b) + \boldsymbol{\xi} \geq \mathbf{e},\ \boldsymbol{\xi} \geq \mathbf{0}, \end{cases} \tag{1}$$

A new data point $\mathbf{x}$ will be classified in class $\mathbf{A}$ if $\text{sgn}(f(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + b) > 0$ and in class $\mathbf{B}$ if $\text{sgn}(f(\mathbf{x})) < 0$.

The main idea of Twin Support Vector Machines (TSVM)[11] is to seek two hyperplanes:

- $f_+(\mathbf{x})(= \mathbf{w}_+^T\mathbf{x} + b_+) = 0$ is closer to class $\mathbf{A}$ and far away from class $\mathbf{B}$,
- $f_-(\mathbf{x})(= \mathbf{w}_-^T\mathbf{x} + b_-) = 0$ is closer to class $\mathbf{B}$ and far away from class $\mathbf{A}$,

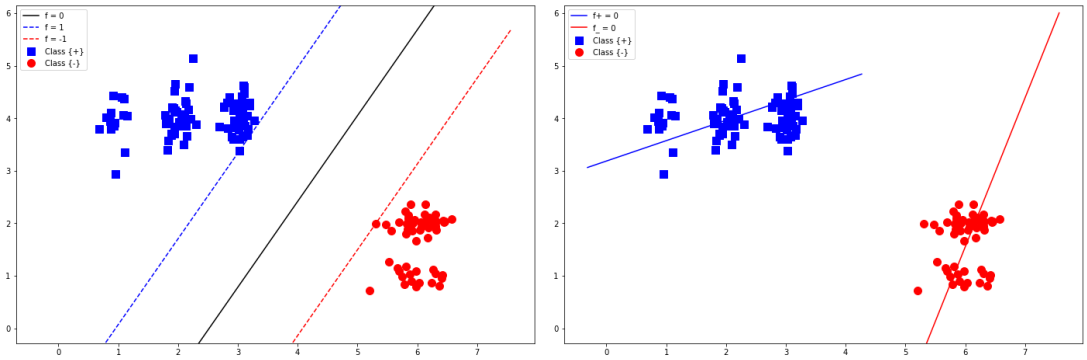
by solving two QPPs as follows:

$$\begin{cases} \min\limits_{\mathbf{w}_+, b_+, \boldsymbol{\xi}} & \frac{1}{2}\|\mathbf{A}\mathbf{w}_+ + \mathbf{e}_A b_+\|^2 + c_1\mathbf{e}_B^T\boldsymbol{\xi}, \\ \text{s.t.} & -(\mathbf{B}\mathbf{w}_+ + \mathbf{e}_B b_+) + \boldsymbol{\xi} \geq \mathbf{e}_B,\ \boldsymbol{\xi} \geq \mathbf{0}, \end{cases} \tag{2}$$

and

$$\begin{cases} \min\limits_{\mathbf{w}_-,b_-,\boldsymbol{\eta}} & \frac{1}{2}\|\mathbf{B}\mathbf{w}_- + \mathbf{e}_B b_-\|^2 + c_2\mathbf{e}_A^T\boldsymbol{\eta}, \\ \text{s.t.} & (\mathbf{A}\mathbf{w}_+ + \mathbf{e}_A b_+) + \boldsymbol{\eta} \geq \mathbf{e}_A,\ \boldsymbol{\eta} \geq \mathbf{0}. \end{cases} \tag{3}$$

A new data $\mathbf{x}$ is classified to class $\mathbf{A}$ or class $\mathbf{B}$ depending on whether it is closer to the hyperplane $f_+(\mathbf{x}) = 0$ or $f_-(\mathbf{x}) = 0$. The SVM and TSVM do not sufficiently exploit structural information with cluster granularity of data, so they describe the distribution structure of two classes being not exactly (see Figure 1).



(a) (b)

Fig. 1. The simple case, in which clusters in each class are constituted by the same trend, the SVM, and TSVM do not exactly describe the distribution trend of data in each class, and don't use information about the number of data points of clusters in each class. (a) SVM, (b) TSVM.

Structural Twin Support Vector Machine (S-TSVM)[12] has two steps: The first step is to extract the structural information within classes. The second step is the model learning. S-TSVM also determines two hyperplanes as TSVM:

$$f_+(\mathbf{x}) = \mathbf{w}_+^T\mathbf{x} + b_+ = 0;\ f_-(\mathbf{x}) = \mathbf{w}_-^T\mathbf{x} + b_- = 0, \tag{4}$$

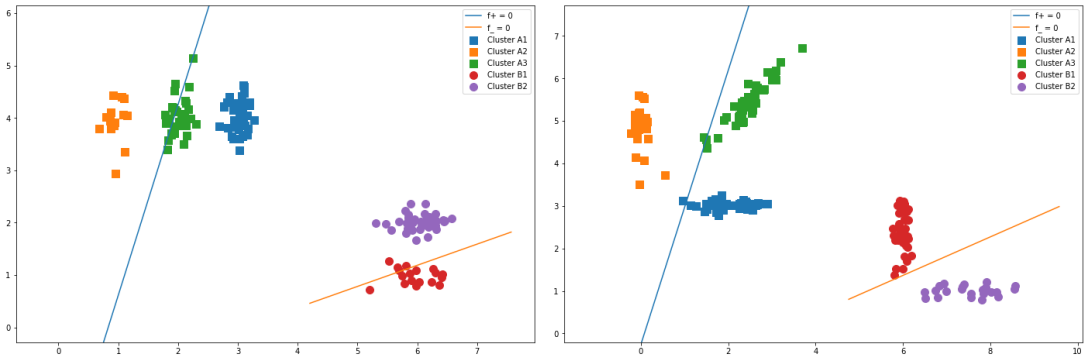
by solving two QPPs as follows:

$$\begin{cases} \min\limits_{\mathbf{w}_+,b_+,\boldsymbol{\xi}} & \frac{1}{2}\|\mathbf{A}\mathbf{w}_+ + \mathbf{e}_A b_+\|^2 + c_1\mathbf{e}_B^T\boldsymbol{\xi} + \frac{1}{2}c_2(\|\mathbf{w}_+\|^2 + b_+^2) + \frac{1}{2}c_3\mathbf{w}_+^T\Sigma_+\mathbf{w}_+, \\ \text{s.t.} & -(\mathbf{B}\mathbf{w}_+ + \mathbf{e}_B b_+) + \boldsymbol{\xi} \geq \mathbf{e}_B,\ \boldsymbol{\xi} \geq \mathbf{0}, \end{cases} \tag{5}$$

$$\begin{cases} \min\limits_{\mathbf{w}_-,b_-,\boldsymbol{\eta}} & \frac{1}{2}\|\mathbf{B}\mathbf{w}_- + \mathbf{e}_B b_-\|^2 + c_4\mathbf{e}_A^T\boldsymbol{\eta} + \frac{1}{2}c_5(\|\mathbf{w}_-\|^2 + b_-^2) + \frac{1}{2}c_6\mathbf{w}_-^T\Sigma_-\mathbf{w}_-, \\ \text{s.t.} & (\mathbf{A}\mathbf{w}_- + \mathbf{e}_A b_-) + \boldsymbol{\eta} \geq \mathbf{e}_A, \boldsymbol{\eta} \geq \mathbf{0}. \end{cases} \tag{6}$$

A new data point is assigned to class $\mathbf{A}$ or class $\mathbf{B}$ in the same manner as in TSVM. The S-TSVM exploits structural information with cluster granularity of one class in each problem. Therefore, the ability of S-TSVM to describe data trends is more accurate than that of TSVM (see Figure 2 in the simple case). However, when data

becomes more complex, the ability to describe data trends of the S-TSVM remains limited (see Figure 2 in complex case).



(c) (d)

Fig. 2. (c) In the simple case, S-TSVM describes quite accurately the distribution trend in each class. (d) In complex cases, S-TSVM has difficulty in describing the distribution trend of data and doesn't use information about the number of data points of clusters in each class.

3. TSVM with Multi-Clusters Data

This section introduces a new method to solve binary classification problems with multi-clusters data: Twin Support Vector Machine with Multi-Clusters Data (called TSVM-MCD). Similar to the S-TSVM,[12] TSVM-MCD also has two steps. The first step is to group data in each class by Ward's linkage clustering method;[15] the second step is model learning. Suppose, there are k clusters in class $\mathbf{A}$, and l clusters in class $\mathbf{B}$. TSVM-MCD uses a cluster-vs-class strategy to determine $(k+l)$ hyperplanes such that each of which is closer to one cluster and far away from the other class. Specifically, the method needs to find k hyperplanes such that the $i-$th hyperplane, $f_{i+}(\mathbf{x}) = \mathbf{w}_{i+}^T\mathbf{x} + b_{i+} = 0, i = 1,\ldots,k$, is closer to cluster $\mathbf{A}_i$ and far away from class $\mathbf{B}$; Also, it needs to find l hyperplanes such that the $j-$th hyperplane, $f_{j-}(\mathbf{x}) = \mathbf{w}_{j-}^T\mathbf{x} + b_{j-} = 0, j = 1,\ldots,l$, is closer to cluster $\mathbf{B}_j$ and far away from class $\mathbf{A}$ (see Figure 3); Here $\mathbf{w}_{i+}, \mathbf{w}_{j-} \in \mathbb{R}^n, b_{i+}, b_{j-} \in \mathbb{R}$.

The classifier is now selected as:

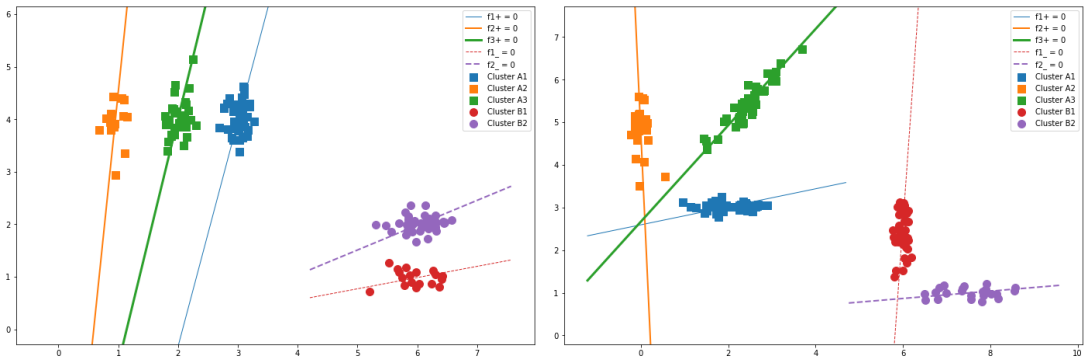
$$f(\mathbf{x}) = \underset{+,\ -}{\operatorname{argmin}}(f_+(\mathbf{x}),\ f_-(\mathbf{x})), \tag{7}$$

with

$$f_+(\mathbf{x}) = \sum_{i=1}^{k} \frac{m_{Ai}}{m_A} f_{i+}(\mathbf{x});\ \ f_-(\mathbf{x}) = \sum_{j=1}^{l} \frac{m_{Bj}}{m_B} f_{j-}(\mathbf{x}). \tag{8}$$

From (8), we can see that $f_+(\mathbf{x})$ is the weighted average of the distances from $\mathbf{x}$ to the hyperplanes $\{f_{i+}(\mathbf{x}) = 0\}$. The $i-$th hyperplane's weight is proportional to

m_{Ai} - the number of data points in the cluster $\mathbf{A}i$. Similarly, $f_-(\mathbf{x})$ is the weighted average of distances from $\mathbf{x}$ to the hyperplanes $\{f_{j-}(\mathbf{x}) = 0\}$. By (7), a new data point $\mathbf{x}$ is classified into class $\mathbf{A}$ or $\mathbf{B}$ depending on whether $f_+(\mathbf{x})$ is less than or greater than $f_-(\mathbf{x})$.



(e) (f)

Fig. 3. The TSVM-MCD exploits structural information with cluster granularity, and information about the number of data points of clusters in each class to model learning. Consequently, the TSVM-MCD can describe the distribution trends of each cluster in each class, so the generalized capability is better than the S-TSVM and TSVM methods. (e) TSVM-MCD in simple case. (f) TSVM-MCD in complex case.

3.1. *The linear case*

When two classes are nearly linear separable, we determine $(k + l)$ hyperplanes in TSVM-MCD by solving $(k + l)$ QPPs as follows:

$$\begin{cases} \min\limits_{\mathbf{w}_{i+},b_{i+},\boldsymbol{\xi}} & \frac{1}{2}\|\mathbf{A}_i\mathbf{w}_{i+} + \mathbf{e}_{Ai}b_{i+}\|^2 + \frac{1}{2}c_1\mathbf{e}_B^T\boldsymbol{\xi} + \frac{1}{2}c_2(\|\mathbf{w}_{i+}\|^2 + b_{i+}^2), \\ \text{s.t.} & (\mathbf{B}\mathbf{w}_{i+} + \mathbf{e}_B b_{i+}) + \boldsymbol{\xi} \geq \mathbf{e}_B, \boldsymbol{\xi} \geq \mathbf{0}, \end{cases} \tag{9}$$

$i = 1, \ldots, k$ and

$$\begin{cases} \min\limits_{\mathbf{w}_{j-},b_{j-},\boldsymbol{\eta}} & \frac{1}{2}\|\mathbf{B}_j\mathbf{w}_{j-} + \mathbf{e}_{Bj}b_{j-}\|^2 + \frac{1}{2}c_3\mathbf{e}_A^T\boldsymbol{\eta} + \frac{1}{2}c_4(\|\mathbf{w}_{j-}\|^2 + b_{j-}^2), \\ \text{s.t.} & (\mathbf{A}\mathbf{w}_{j-} + \mathbf{e}_A b_{j-}) + \boldsymbol{\eta} \geq \mathbf{e}_A, \boldsymbol{\eta} \geq \mathbf{0}, \end{cases} \tag{10}$$

$j = 1, \ldots, l$.

Here, $\mathbf{e}_{Ai} \in \mathbb{R}^{m_{Ai}\times 1}$, $\mathbf{e}_{Bj} \in \mathbb{R}^{m_{Bj}\times 1}$, $\mathbf{e}_A \in \mathbb{R}^{m_A\times 1}$, and $\mathbf{e}_B \in \mathbb{R}^{m_B\times 1}$ are vectors of ones. $\boldsymbol{\eta} \in \mathbb{R}^{m_A\times 1}$, and $\boldsymbol{\xi} \in \mathbb{R}^{m_B\times 1}$ are vectors of slack variables. c_1, c_2, c_3, c_4 are penalty coefficients. In the problem (9), $\|\mathbf{A}_i\mathbf{w}_{i+} + \mathbf{e}_{Ai}b_{i+}\|^2$ is the sum of squares of distances from data points in cluster $\mathbf{A}_i$ to the hyperplane $f_{i+}(\mathbf{x}) = 0$, and it takes structural information with cluster granularity. Therefore, we do not need to add the $\frac{1}{2}c_3\mathbf{w}_+^T\Sigma_+\mathbf{w}_+$ term as in S-TSVM. $\frac{1}{2}c_1\mathbf{e}_B^T\boldsymbol{\xi}$ is the sum of errors, $\frac{1}{2}c_2(\|\mathbf{w}_{i+}\|^2 + b_{i+}^2)$

is the regularization term. The constraints of problem (9) are defined by the points of class **B**. The problem (10) is similarly established for clusters $\mathbf{B}_j$ of class **B** with the constraints defined by class **A**.

We will solve two problems (9), and (10) by solving two dual problems. Specifically, the Lagrange function of (9) is given by:

$$\mathcal{L}(\mathbf{w}_{i+}, b_{i+}, \boldsymbol{\xi}, \boldsymbol{\alpha}, \boldsymbol{\beta}) = \frac{1}{2}\|\mathbf{A}_i\mathbf{w}_{i+} + \mathbf{e}_{Ai}b_{i+}\|^2 + c_1\mathbf{e}_B^T\boldsymbol{\xi} + \frac{1}{2}c_2(\|\mathbf{w}_{i+}\|^2 + b_{i+}^2) - \boldsymbol{\alpha}^T((\mathbf{B}\mathbf{w}_{i+} + \mathbf{e}_B b_{i+}) + \boldsymbol{\xi} - \mathbf{e}_B) - \boldsymbol{\beta}^T\boldsymbol{\xi}. \tag{11}$$

From the (Theorem 2.1), the KKT system of (9) is as follows:

$$\mathbf{A}_i^T(\mathbf{A}_i\mathbf{w}_{i+} + \mathbf{e}_{Ai}b_{i+}) + c_2\mathbf{w}_{i+} - \mathbf{B}^T\boldsymbol{\alpha} = \mathbf{0}, \tag{12}$$

$$\mathbf{e}_{Ai}^T(\mathbf{A}_i\mathbf{w}_{i+} + \mathbf{e}_{Ai}b_{i+}) + c_2 b_{i+} - \mathbf{e}_B^T\boldsymbol{\alpha} = 0, \tag{13}$$

$$c_1\mathbf{e}_B - \boldsymbol{\alpha} - \boldsymbol{\beta} = \mathbf{0}, \tag{14}$$

$$\boldsymbol{\alpha}^T((\mathbf{B}\mathbf{w}_{i+} + \mathbf{e}_B b_{i+}) + \boldsymbol{\xi} - \mathbf{e}_B) = \mathbf{0},\ \boldsymbol{\beta}^T\boldsymbol{\xi} = 0. \tag{15}$$

Defining $\mathbf{H}_i = [\mathbf{A}_i, \mathbf{e}_{Ai}]$, $\mathbf{G} = [\mathbf{B}, \mathbf{e}_B]$, $\mathbf{z}_{i+}^T = [\mathbf{w}_{i+}^T, b_{i+}]$, $i = 1, \ldots, k$, and $\mathbf{I}$ is the identity matrix of order $(n+1)$, from (12) and (13) we have

$$\mathbf{H}_i^T\mathbf{H}_i\mathbf{z}_{i+} + c_2\mathbf{I}\mathbf{z}_{i+} - \mathbf{G}^T\boldsymbol{\alpha} = \mathbf{0} \tag{16}$$

$$\Rightarrow \left[\mathbf{H}_i^T\mathbf{H}_i + c_2\mathbf{I}\right]\mathbf{z}_{i+} = \mathbf{G}^T\boldsymbol{\alpha} \tag{17}$$

$$\Rightarrow \mathbf{z}_{i+} = \left[\mathbf{H}_i^T\mathbf{H}_i + c_2\mathbf{I}\right]^{-1}\mathbf{G}^T\boldsymbol{\alpha}. \tag{18}$$

Substituting (18) into the Lagrangian (11), and combined with the conditions (14), and (15) we have the dual problem of (9) as follows:

$$\begin{cases} \max\limits_{\boldsymbol{\alpha}} & \mathbf{e}_B^T\boldsymbol{\alpha} - \frac{1}{2}\boldsymbol{\alpha}^T\mathbf{G}[\mathbf{H}_i^T\mathbf{H}_i + c_2\mathbf{I}]^{-1}\mathbf{G}^T\boldsymbol{\alpha}, \\ \text{s.t.} & \mathbf{0} \le \boldsymbol{\alpha} \le c_1\mathbf{e}_B. \end{cases} \tag{19}$$

In a similar way, by defining $\mathbf{G}_j = [\mathbf{B}_j, \mathbf{e}_{Bj}]$, $\mathbf{H} = [\mathbf{A}, \mathbf{e}_A]$, $\mathbf{z}_{j-}^T = [\mathbf{w}_{j-}^T, b_{j-}]$, $j = 1, \ldots, l$, we obtain the solutions of problem (10):

$$\mathbf{z}_{j-} = \left[\mathbf{G}_j^T\mathbf{G}_j + c_4\mathbf{I}\right]^{-1}\mathbf{H}^T\boldsymbol{\gamma}, \tag{20}$$

where $\boldsymbol{\gamma}$ is the solution of the dual problem of (10) as follows:

$$\begin{cases} \max\limits_{\boldsymbol{\gamma}} & \mathbf{e}_A^T\boldsymbol{\gamma} - \frac{1}{2}\boldsymbol{\gamma}^T\mathbf{H}[\mathbf{G}_j^T\mathbf{G}_j + c_4\mathbf{I}]^{-1}\mathbf{H}^T\boldsymbol{\gamma}, \\ \text{s.t.} & \mathbf{0} \le \boldsymbol{\gamma} \le c_3\mathbf{e}_A. \end{cases} \tag{21}$$

3.2. *The nonlinear case*

The linear TSVM-MCD can also easily be extended when two classes are nonlinearly separable. Let $\Phi : \mathbb{R}^n \to \mathbb{H}$ be a nonlinear mapping, where $\mathbb{H}$ is a Hilbert space whose dimension is not less than n (maybe infinite-dimensional). Since $\mathbb{S} = \text{span}(\Phi(\mathbf{C}^T))$ is a subspace of $\mathbb{H}$ whose dimension does not exceed m, we can consider $\mathbb{S}$ as an Euclidean space and $\Phi : \mathbb{R}^n \to \mathbb{S}$. Suppose that after the clustering step on space $\mathbb{S}$, we obtain k clusters $\Phi(\mathbf{A}_1), \ldots, \Phi(\mathbf{A}_k)$ in the class $\Phi(\mathbf{A})$, each cluster $\Phi(\mathbf{A}_i)$ consists of m_{Ai} data points; and l clusters $\Phi(\mathbf{B}_1), \ldots, \Phi(\mathbf{B}_l)$ in the class $\Phi(\mathbf{B})$, each cluster $\Phi(\mathbf{B}_j)$ consists of m_{Bj} data points. In space $\mathbb{S}$, a hyperplane $\Phi(\mathbf{x}^T)\mathbf{h} + b = 0$ (with $\mathbf{h} \in \mathbb{S}$ being the normal vector) can be rewritten as $\Phi(\mathbf{x}^T)\Phi(\mathbf{C}^T)\mathbf{u} + b = 0$ for some vector $\mathbf{u} \in \mathbb{R}^m$. Therefore, by defining $\Phi(\mathbf{x}^T)\Phi(\mathbf{C}^T) = K(\mathbf{x}^T, \mathbf{C}^T)$, the hyperplane has the form $K(\mathbf{x}^T, \mathbf{C}^T)\mathbf{u} + b = 0$, K is a predefined kernel.[16]

TSVM-MCD determines k hyperplanes such that the $i-$th one: $K(\mathbf{x}^T,\ \mathbf{C}^T)\mathbf{u}_{i+} + b_{i+} = 0$ is closer to cluster $\Phi(\mathbf{A}_i)$ and far away from class $\Phi(\mathbf{B})$. It also determines l hyperplanes such that the $j-$th one: $K(\mathbf{x}^T,\ \mathbf{C}^T)\mathbf{u}_{j-} + b_{j-} = 0$ is closer to cluster $\Phi(\mathbf{B}_j)$ and far away from class $\Phi(\mathbf{A})$. Specifically, we have $(k + l)$ QPPs as follows:

$$\begin{cases} \min\limits_{\mathbf{u}_{i+}, b_{i+}, \boldsymbol{\xi}} & \frac{1}{2}\|K(\mathbf{A}_i, \mathbf{C}^T)\mathbf{u}_{i+} + \mathbf{e}_{Ai}b_{i+}\|^2 + \frac{c_1}{2}\mathbf{e}_B^T\boldsymbol{\xi} + \frac{c_2}{2}(\|\mathbf{u}_{i+}\|^2 + b_{i+}^2), \\ \text{s.t.} & (K(\mathbf{B}, \mathbf{C}^T)\mathbf{u}_{i+} + \mathbf{e}_B b_{i+}) + \boldsymbol{\xi} \geq \mathbf{e}_B, \boldsymbol{\xi} \geq \mathbf{0}; \end{cases} \tag{22}$$

$\mathbf{u}_{i+} \in \mathbb{R}^m$, $i = 1, \ldots, k$ and

$$\begin{cases} \min\limits_{\mathbf{u}_{j-}, b_{j-}, \boldsymbol{\eta}} & \frac{1}{2}\|K(\mathbf{B}_j, \mathbf{C}^T)\mathbf{u}_{j-} + \mathbf{e}_{Bj}b_{j-}\|^2 + \frac{c_3}{2}\mathbf{e}_A^T\boldsymbol{\eta} + \frac{c_4}{2}(\|\mathbf{u}_{j-}\|^2 + b_{j-}^2), \\ \text{s.t.} & (K(\mathbf{A}, \mathbf{C}^T)\mathbf{u}_{j-} + \mathbf{e}_A b_{j-}) + \boldsymbol{\eta} \geq \mathbf{e}_A, \boldsymbol{\eta} \geq \mathbf{0}; \end{cases} \tag{23}$$

$\mathbf{u}_{j-} \in \mathbb{R}^m$, $j = 1, \ldots, l$.

In an exactly similar way such as the linear case, two dual problems of (22) and (23) are as follows:

$$\begin{cases} \max\limits_{\boldsymbol{\alpha}} & \mathbf{e}_B^T\boldsymbol{\alpha} - \frac{1}{2}\boldsymbol{\alpha}^T\mathbf{G}[\mathbf{H}_i^T\mathbf{H}_i + c_2\mathbf{I}]^{-1}\mathbf{G}^T\boldsymbol{\alpha}, \\ \text{s.t.} & \mathbf{0} \leq \boldsymbol{\alpha} \leq c_1\mathbf{e}_B, \end{cases} \tag{24}$$

and

$$\begin{cases} \max\limits_{\boldsymbol{\gamma}} & \mathbf{e}_A^T\boldsymbol{\gamma} - \frac{1}{2}\boldsymbol{\gamma}^T\mathbf{H}[\mathbf{G}_j^T\mathbf{G}_j + c_4\mathbf{I}]^{-1}\mathbf{H}^T\boldsymbol{\gamma}, \\ \text{s.t.} & \mathbf{0} \leq \boldsymbol{\gamma} \leq c_3\mathbf{e}_A. \end{cases} \tag{25}$$

Where, $\mathbf{H}_i = [K(\mathbf{A}_i, \mathbf{C}^T), \mathbf{e}_{Ai}]$, $\mathbf{G} = [K(\mathbf{B}, \mathbf{C}^T), \mathbf{e}_B]$, $\mathbf{G}_j = [K(\mathbf{B}_j, \mathbf{C}^T), \mathbf{e}_{Bj}]$, $\mathbf{H} = [K(\mathbf{A}, \mathbf{C}^T), \mathbf{e}_A]$, and we have solutions of (22), (23) as follows:

$$\mathbf{z}_{i+} = \left[\mathbf{H}_i^T\mathbf{H}_i + c_2\mathbf{I}\right]^{-1}\mathbf{G}^T\boldsymbol{\alpha}, i = \overline{1, k}, \tag{26}$$

$$\mathbf{z}_{j-} = \left[\mathbf{G}_j^T\mathbf{G}_j + c_4\mathbf{I}\right]^{-1}\mathbf{H}^T\boldsymbol{\gamma}, j = \overline{1, l}, \tag{27}$$

here, $\mathbf{z}_{i+}^T = [\mathbf{u}_{i+}^T, b_{i+}]$ $\mathbf{z}_{j-}^T = [\mathbf{u}_{j-}^T, b_{j-}]$, and $\mathbf{I}$ is the identity matrix of order $(m+1)$.

The classification function is now selected as:

$$f(\mathbf{x}) = \underset{+,\ -}{\operatorname{argmin}}(f_+(\mathbf{x}),\ f_-(\mathbf{x})), \tag{28}$$

with

$$\begin{cases} f_+(\mathbf{x}) = \sum\limits_{i=1}^{k} \dfrac{m_{Ai}}{m_A}(K(\mathbf{x}^T, \mathbf{C}^T)\mathbf{u}_{i+} + b_{i+}); \\ f_-(\mathbf{x}) = \sum\limits_{j=1}^{l} \dfrac{m_{Bj}}{m_B}(K(\mathbf{x}^T, \mathbf{C}^T)\mathbf{u}_{j-} + b_{j-}). \end{cases} \tag{29}$$

4. Experiments

In this section, we compare the training time, tested accuracy, and 10-fold cross-validated accuracy (10-fold CV) of TSVM-MCD against S-TSVM[12] and TSVM[11] on various UCI data sets.[17] All algorithms are settled by Python programming language and run on a desktop with an Intel Xeon E5, and 32GB RAM. All settings are uploaded to

- https://github.com/makeho8/Algorithms.

We implement these algorithms on UCI data sets[17] which have been experimented in.[11,12] We randomly selected 70% of each extracted data set for training and 30% for testing. We both used 10-fold cross-validation (CV) on the training set and tested accuracy on the testing set to evaluate the performance of all algorithms. All hyper-parameters such as c_1, c_2 of TSVM, $c_1, c_2, c_3, c_4, c_5, c_6$ of S-TSVM, c_1, c_2, c_3, c_4 of TSVM-MCD, and γ of RBF kernel are set to 1 to balance the roles of components in the QPP's objective functions of all algorithms.

Table 1 compares tested accuracy, and 10-fold CV accuracy with linear kernel between TSVM-MCD, S-TSVM, and TSVM on 9 small UCI data sets. Because the data sets are small, the training time of all algorithms is not much different, so we don't show the time in Table 1. From Table 1 we can see that the generalization performance of TSVM-MCD is better than that of TSVM and S-TSVM, it is expressed in tested accuracy. The tested accuracy of TSVM-MCD is higher than that of other algorithms in most cases. The 10-fold CV accuracy of the algorithms is comparable and quite close to the tested accuracy. This shows that the TSVM-MCD algorithm is quite stable, not falling into the case of over-fitting and under-fitting with training data sets.

Table 2 compares the training time, tested accuracy, and 10-fold CV accuracy with RBF kernel between TSVM-MCD, S-TSVM, and TSVM on 6 small UCI data sets. From Table 2 we can see that the training time of TSVM-MCD and S-TSVM are slower than that of TSVM for the nonlinear case of all 6 data sets. This is because the S-TSVM and TSVM-MCD have to cluster the data and process the problem on each cluster. The training time of TSVM-MCD is faster than that of

Table 1. Training time (s), tested accuracy (%), and 10-fold cross-validated accuracy (%) with a linear Kernel of TSVM, S-TSVM, and TSVM-MCD on UCI data sets.

Data sets	Algorithms		
	TSVM	S-TSVM	TSVM-MCD
$(m \times n)$	Test(%)	Test(%)	Test(%)
$(k \times l)$	10-fold CV (%)	10-fold CV (%)	10-fold CV (%)
Hepatitis	87.2	87.2	**89.4**
(155×19)	81.7 +/- 12.1	81.7 +/- 12.1	82.5 +/- 11.0
(2×1)			
Liver-disorders	77.9	77.9	**79.8**
(345×5)	73.4 +/- 8.2	73.4 +/- 8.2	75.9 +/- 8.5
(1×2)			
Ionosphere	88.7	88.7	88.7
(351×34)	86.9 +/- 7.9	87.4 +/- 7.6	87.4 +/- 7.6
(1×1)			
Glioma-grading	85.3	85.3	**86.1**
(839×25)	87.7 +/- 4.8	87.7 +/- 4.8	87.1 +/- 4.6
(2×2)			
Auto-mpg	90.0	90.0	90.0
(398×7)	90.7 +/- 4.8	90.7 +/- 4.8	89.9 +/- 4.4
(1×1)			
Automobile	90.3	90.3	**93.5**
(205×25)	84.6 +/- 10.0	84.6 +/- 10.0	80.4 +/- 11.0
(1×2)			
Heart-disease	81.3	81.3	81.3
(303×13)	82.9 +/- 7.2	82.9 +/- 7.2	80.1 +/- 7.7
(1×1)			
Heart-failure	78.9	78.9	77.8
(299×12)	84.7 +/- 9.9	84.7 +/- 9.9	82.8 +/- 10.9
(2×1)			
Credit-approval	84.1	84.1	84.1
(690×46)	86.3 +/- 2.8	86.3 +/- 2.8	84.1 +/- 6.1
(1×1)			

Where m is the data point number of each data set, n is the dimension of the data, k is the number of clusters in the class **A**, and l is the number of clusters in class **B**, respectively.

S-TSVM because the S-TSVM must calculate the covariance matrices of all clusters in two classes. That is the cost to obtain a more precise classification. We can see that the classification accuracy of TSVM-MCD, and S-TSVM are better than that

of TSVM in most data sets.

Note that, the number of clusters ($k \times l$, k is the number of clusters in the class $\{+\}$ and l is in the class $\{-\}$) in each class (shows in Table 1 and Table 2) are auto-detected by using elbow method.

Table 2. Training time (s), tested accuracy (%), and 10-fold cross-validated accuracy (%) with an RBF Kernel of TSVM, S-TSVM, and TSVM-MCD on UCI data sets

Data sets	Algorithms		
	TSVM	S-TSVM	TSVM-MCD
$(m \times n)$	Test(%)	Test(%)	Test(%)
$(k \times l)$	10-fold CV (%)	10-fold CV (%)	10-fold CV (%)
	Time (s)	Time (s)	Time (s)
Liver-disorders	79.8	79.8	**81.7**
(345×5)	79.2 +/- 5.9	75.9 +/- 8.3	75.1 +/- 7.9
(1×2)	1.40	3.55	2.56
Ionosphere	86.8	91.5	91.5
(351×34)	84.8 +/- 9.2	95.5 +/- 3.4	95.5 +/- 4.2
(1×1)	1.27	3.29	1.80
Glioma-grading	77.0	83.3	**84.1**
(839×25)	70.9 +/- 5.8	85.5 +/- 5.3	85.5 +/- 6.8
(2×2)	7.58	20.02	16.29
Auto-mpg	91.7	91.7	91.7
(398×7)	91.0 +/- 4.3	90.7 +/- 3.6	89.2 +/- 4.8
(1×1)	1.69	4.50	2.39
Heart-disease	73.6	76.9	76.9
(303×13)	71.1 +/- 11.5	83.0 +/- 8.1	82.0 +/- 5.6
(1×1)	0.99	2.46	1.62
Credit-approval	69.6	85.0	85.0
(690×46)	68.8 +/- 5.0	85.7 +/- 4.0	81.8 +/- 4.5
(1×1)	4.82	12.95	8.69

5. Conclusion

This paper proposes a new Twin Support Vector Machine with Multi-Clusters Data (TSVM-MCD) for binary classification problems, using a cluster-vs-class strategy. TSVM-MCD has two steps: The first step is grouping in each class by Ward's linkage clustering method; The second is model learning. The classifier is based on weighted average distances from the data point to the cluster's representative hyperplanes. TSVM-MCD has a slower execution time than that of TSVM, but faster than S-TSVM in nonlinear cases. Regarding classification accuracy, TSVM-MCD is better

than TSVM, and S-TSVM in most data sets for both linear and nonlinear cases. For binary classification problems with multi-clusters data, in which each class contains many clusters, and each cluster has individual distribution trends and data points, the TSVM-MCD algorithm is more effective in generalized performance. This new method may not be suitable for multi-classes problems. However, it seems useful in solving the classification problem with imbalanced data.

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