

Sparse Twin Support Vector Clustering using Pinball Loss

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Abstract—Clustering is a widely used machine learning technique for unlabelled data. One of the recently proposed techniques is the twin support vector clustering (TWSVC) algorithm. The idea of TWSVC is to generate hyperplanes for each cluster. TWSVC utilizes the hinge loss function to penalize the misclassification. However, the hinge loss relies on shortest distance between different clusters, and is unstable for noise-corrupted datasets, and for re-sampling. In this paper, we propose a novel Sparse Pinball loss Twin Support Vector Clustering (SPTSVC). The proposed SPTSVC involves the ϵ -insensitive pinball loss function to formulate a sparse solution. Pinball loss function provides noise-insensitivity and re-sampling stability. The ϵ -insensitive zone provides sparsity to the model and improves testing time. Numerical experiments on synthetic as well as real world benchmark datasets are performed to show the efficacy of the proposed model. An analysis on the sparsity of various clustering algorithms is presented in this work. In order to show the feasibility and applicability of the proposed SPTSVC on biomedical data, experiments have been performed on epilepsy and breast cancer datasets.

Index Terms—TWSVC, SVM, pinball loss, quantile distance, sparsity, noise insensitivity, noisy data.

I. INTRODUCTION

SUPPORT vector machines (SVMs) have proven to be one of the most accurate classification techniques in the past few decades [1]. The solution of SVM involves a quadratic programming problem (QPP) to generate a classifying hyperplane. SVM and its variants have been applied in various applications such as Alzheimer's disease [2], [3], image classification [4], investor sentiment classification [5], EEG classification [6], and breast cancer [7]. The solution of SVM requires the solution of a QPP of large size. This incurs high computation time for the SVM algorithm. In order to reduce the computational complexity of SVM, Jayadeva et al. [8] proposed a novel technique termed as twin support vector machine (TWSVM). In TWSVM, instead of one large QPP, two small QPPs are solved to generate twin hyperplanes. Shao et al. [9] proposed a twin bounded support vector machine (TBSVM) to embody the structural risk minimization principle (SRM) of statistical theory in TWSVM. The SRM principle is introduced in TBSVM by including a regularization term in the objective function of TWSVM. Some twin SVM based models

are proposed for multiclass classification [10] as well. Tanveer [11] used a smoothing technique to propose a smooth linear programming TWSVM (SLPTSVM). It leads to unconstrained optimization problems, which in turn reduces the computation cost. The smoothing function is used to approximate the loss, and makes it differentiable. Moreover, Newton method is used to propose an iterative implicit Lagrangian TWSVM algorithm [12]. Another improvement over SVM is proposed as least squares twin support vector machine (LSTSVM) [13], which only involves linear equations in the solution. An energy-based LSTSVM (RELS-TSVM) [14] performed well on benchmark datasets in a recent survey [15].

To reduce the effect of noise in SVM, various techniques have been proposed, such as fuzzy based techniques [16], [17]. To improve the noise insensitivity, Huang et al. [18] proposed a pinball loss function for SVM. More efficient models based on pinball loss are also proposed in the past. A twin parametric-margin SVM using pinball loss (Pin-TPMSVM) is also proposed [19], based on the twin parametric-margin approach. This leads to decrease in computational time of pin-SVM algorithm. Recently, a general pinball twin SVM (Pin-GTSVM) was proposed for pattern classification. The Pin-GTSVM model is in the spirit of the original TWSVM model of classification, rather than the parametric version as in [19]. In order to include sparsity in the Pin-GTSVM, Tanveer et al. [20] proposed a sparse pinball twin support vector machine (SPTWSVM). The solution of SPTWSVM is sparser than Pin-GTSVM. This leads to better generalization performance in SPTWSVM with lesser testing time. By including the SRM principle in Pin-GTSVM, an improved sparse pinball twin support vector machine (ISPTSVM) [21] is proposed to improve the generalization performance. However, most of these pinball loss based models have been used for classification problems.

Clustering algorithms are very useful in real world applications, since a large amount of data is unlabelled in nature. Many algorithms are proposed for clustering in the past [22]. Support vector clustering (SVC) is proposed [23] for unlabelled data. An efficient formulation termed as twin support vector clustering (TWSVC) [24] is proposed using the concave-convex programming (CCCP). To improve the computation time, a fuzzy based least squares TWSVC (FLSTWSVC) is formulated [25]. However, the additional fuzzy function in FLSTWSVC incurs additional computational cost. To include the SRM principle in clustering algorithms, a twin bounded support vector clustering (TBSVC) [26] was proposed, using additional regularization term in the formulation of TWSVC. Further, a ramp loss based twin support vector

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clustering (RampTWSVC) [27] is proposed to bring robustness to classifier, in presence of points lying far away from their clusters. RampTWSVC utilises the within class and between class scatter information to improve the noise insensitivity. However, the ramp loss function is non-convex in nature. Recently, a least squares projection twin SVC (LSPTSVC) [28] is proposed, where the intra-class scatter is minimized, and inter-class scatter is maximized in the formulation. To include the pinball loss in the optimization problem of twin SVM based clustering algorithms, a pinball loss based twin support vector clustering (pinTSVC) [29] algorithm is proposed. This lead to improvement in the noise insensitivity of the clustering algorithm.

However, the generalization performance of SVM based models is determined by the sparsity of the solution obtained. Classifiers with higher sparsity level often give better generalization performance [20]. In order to include sparsity with noise insensitivity, motivated by the works on pinball twin SVM and TWSVC, we propose a novel sparse twin support vector clustering using pinball loss (SPTSVC). The formulation of proposed SPTSVC involves a ϵ -insensitive pinball loss function to construct the clustering hyperplanes. The proposed SPTSVC solves the optimization problem with sparser solution compared to existing algorithms, while still enjoying properties of noise-insensitivity and re-sampling stability. The main contributions of our paper are as follows:

- A novel sparse pinball loss twin support vector clustering algorithm is proposed for noisy data.
- The proposed SPTSVC is insensitive to noisy data. Further, it is stable for re-sampling which is required for large scale datasets. Thus its applicable to various real world problems.
- The proposed SPTSVC leads to sparse solution to the optimization problem, thereby reducing testing time.
- An analysis on the sparsity of proposed and existing algorithms is presented in this work.
- Biomedical applications are presented for clustering by using image and time-series data.

We have organized the paper as follows: Section II gives brief description of recent works on clustering. In Section III, formulation of the proposed algorithm has been provided. Section IV discusses the advantages of the proposed SPTSVC model, while the experimental results are given in Section V. Section VI shows the applicability of the proposed model on biomedical data. The conclusions with future work are given in Section VII.

II. BACKGROUND

In this paper, m denotes the number of samples. Each sample has n number of features. Hence, every data sample of a dataset can be represented as $x_i = (x_i^1, x_i^2, \dots, x_i^n)$ for $i = 1, 2, \dots, m$.

Suppose there are k clusters. Then for $i = 1, 2, \dots, k$, matrix X_i of dimensions $m_i \times n$ contains all points in the i^{th} cluster. Rest of the points are collected in matrix $\hat{X}_i$ of dimensions $(m - m_i) \times n$. All vectors are column vectors, L_2 norm is denoted as $\|\cdot\|$, and e represents vector of ones of appropriate dimension.

A. TWSVC

Based on the principles of TWSVM, TWSVC is proposed by Shao et al. [24]. TWSVC [24] obtains k cluster center planes $\omega_i^T x + b_i = 0, i = 1, \dots, k$. These cluster center planes are obtained by solving the following optimization problem:

$$\begin{aligned} \min_{\omega_i, b_i, \xi_i} \quad & \frac{1}{2} \|X_i \omega_i + b_i e\|^2 + c e^T \xi_i \\ \text{s.t.} \quad & |\hat{X}_i \omega_i + b_i e| \geq e - \xi_i, \xi_i \geq 0, \end{aligned} \quad (1)$$

here $c > 0$ is the penalty parameter, and ξ_i is the slack variable for bounding the error term.

From this formulation one can observe that the i^{th} cluster center plane is close to the points X_i and far away from the points $\hat{X}_i$. Shao et al. [24] showed that the above optimization problem can be decomposed into smaller convex quadratic sub-problems using concave-convex procedure (CCCP) [30] technique, which can then be optimized using Karush–Kuhn–Tucker (KKT) conditions [31].

$$\begin{aligned} \min_{\omega_i^{j+1}, b_i^{j+1}, \xi_i^{j+1}} \quad & \frac{1}{2} \|X_i \omega_i^{j+1} + b_i^{j+1} e\|^2 + c e^T \xi_i^{j+1} \\ \text{s.t.} \quad & T(|\hat{X}_i \omega_i^{j+1} + b_i^{j+1} e|) \geq e - \xi_i^{j+1}, \xi_i^{j+1} \geq 0, \end{aligned} \quad (2)$$

where $j = 0, 1, 2, \dots$ is the index of successive sub-problems and c is the same penalty parameter. $T(\cdot)$ denotes the first order Taylor expansion. The sub-gradient of $|\hat{X}_i \omega_i^{j+1} + b_i^{j+1} e|$ can be calculated as $\text{diag}(\text{sign}(\hat{X}_i \omega_i^j + b_i^j e))$, resulting in the following:

$$T(|\hat{X}_i \omega_i^{j+1} + b_i^{j+1} e|) = Z_i (\hat{X}_i \omega_i^{j+1} + b_i^{j+1} e), \quad (3)$$

$$Z_i = \text{diag}(\text{sign}(\hat{X}_i \omega_i^j + b_i^j e)). \quad (4)$$

The solution to (2) can be obtained by solving its dual form. Using Karush–Kuhn–Tucker (KKT) conditions [31], we get the dual problem as:

$$\begin{aligned} \min_{\alpha} \quad & \frac{1}{2} \alpha^T G (H^T H)^{-1} G^T \alpha - e^T \alpha \\ \text{s.t.} \quad & 0 \leq \alpha \leq c e, \end{aligned} \quad (5)$$

where $G = Z_i [\hat{X}_i \ e]$, $H = [X_i \ e]$, and $\alpha \in R^{m-m_i}$ is the Lagrangian multiplier vector. After the solution of (5) is obtained, we obtain cluster plane parameters $[\omega_i^{j+1}, b_i^{j+1}] = (H^T H)^{-1} G^T \alpha$.

B. Loss function

Pinball loss function [18] is defined as:

$$\mathcal{L}_{\tau}(u) = \begin{cases} u & u \geq 0, \\ -\tau u & u < 0, \end{cases}$$

here $\tau \in [0, 1]$. When $u < 0$, we still obtain a small penalty as opposed to zero penalty in hinge loss. Therefore, there is a smaller penalty for correctly classified points as

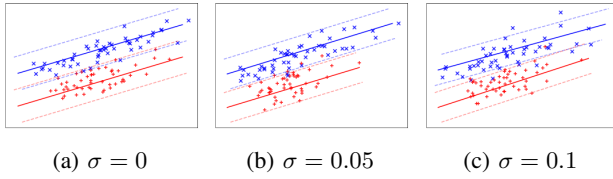


Fig. 1: Plot showing different formation of clusters by linear SPTSVC for a two-dimensional dataset corrupted with Gaussian noise having zero-mean and σ standard deviation.

well. This places an upper bound on the number of errors at decision boundaries, thus providing insensitivity to feature noise. However, since sub-gradient of pinball loss function is non-zero everywhere except origin, it leads to losing sparsity of the solution. To counter this limitation, ϵ -insensitive pinball loss function [18] can be used:

$$\mathcal{L}_\tau^\epsilon(u) = \begin{cases} u - \epsilon & u > \epsilon, \\ 0 & -\frac{\epsilon}{\tau} \leq u \leq \epsilon \\ -\tau(u + \frac{\epsilon}{\tau}) & u < -\frac{\epsilon}{\tau}, \end{cases}$$

In range $[-\frac{\epsilon}{\tau}, \epsilon]$, the sub-gradient of the ϵ -insensitive pinball loss function is 0, thereby leading to sparsity. In this ϵ -insensitive zone of width $\epsilon(1 + \frac{1}{\tau})$, no penalty is given to any data point. This allows us to achieve both noise-insensitivity and sparsity at the same time.

III. PROPOSED SPARSE PINBALL LOSS TWIN SUPPORT VECTOR CLUSTERING (SPTSVC)

We utilize the sparse pinball loss function to incorporate the property of noise-insensitivity and sparsity in the TWSVC formulation. In this section, we propose a Sparse Pinball loss Twin Support Vector Clustering (SPTSVC) algorithm for linear and non-linear cases.

A. Linear SPTSVC

The proposed linear SPTSVC seeks k cluster-center planes $[\omega_i, b_i]$, $i = 1, \dots, k$ by obtaining solution of the following optimization problem:

$$\begin{aligned} \min_{\omega_i, b_i, \xi_i} \quad & \frac{1}{2} \|X_i \omega_i + b_i e\|^2 + c e^T \xi_i \\ \text{s.t.} \quad & |\hat{X}_i \omega_i + b_i e| \geq e - \xi_i - e\epsilon, \\ & |\hat{X}_i \omega_i + b_i e| \leq e + \frac{\xi_i}{\tau} + e\frac{\epsilon}{\tau} \\ & \xi_i \geq 0, \end{aligned} \quad (6)$$

here ξ_i is the slack variable, $\tau \in [0, 1]$ and $\epsilon \in [0, 1]$ are the parameters of sparse pinball loss function. The first term of objective function seeks to minimize the sum of squared distance of points in X_i from hyperplane $[\omega_i; b_i]$. The second term ξ_i is the slack variable. The first and second constraints seeks to minimize the penalty arising from points in $\hat{X}_i$ within $1 - \epsilon$ unit distance from hyperplane $[\omega_i; b_i]$, and also the points which are at-least $1 + \frac{\epsilon}{\tau}$ distance away from hyperplane $[\omega_i; b_i]$.

The third constraint makes sure that the slack variable remains positive. Therefore, a tube of width $\epsilon(1 + \frac{1}{\tau})$ exists where we do not penalise the points at all. For illustrating the robustness of SPTSVC to noise, we have shown the clusters formed for a two-dimensional sample dataset consisting of two classes '+' and 'x' in Fig. 1.

We now utilize the CCCP [30] technique to break the i^{th} problem into smaller convex quadratic programming sub-problems.

$$\begin{aligned} \min_{\omega_i^{j+1}, b_i^{j+1}, \xi_i^{j+1}} \quad & \frac{1}{2} \|X_i \omega_i^{j+1} + b_i^{j+1} e\|^2 + c e^T \xi_i^{j+1} \\ \text{s.t.} \quad & T(|\hat{X}_i \omega_i^{j+1} + b_i^{j+1} e|) \geq e - \xi_i^{j+1} - e\epsilon, \\ & T(|\hat{X}_i \omega_i^{j+1} + b_i^{j+1} e|) \leq e + \frac{\xi_i^{j+1}}{\tau} + e\frac{\epsilon}{\tau} \\ & \xi_i^{j+1} \geq 0. \end{aligned} \quad (7)$$

Using first order Taylor series expansion we get:

$$T(|\hat{X}_i \omega_i^{j+1} + b_i^{j+1} e|) = Z_i(\hat{X}_i \omega_i^{j+1} + b_i^{j+1} e), \quad (8)$$

where:

$$Z_i = \text{diag}(\text{sign}(\hat{X}_i \omega_i^j + b_i^j e)). \quad (9)$$

The above optimization problem is the primal formulation of SPTSVC. It can be observed that (7) is similar to TWSVC primal, with the difference in the constraints. This is due to the change in the loss function of the problem. We then convert the primal to its corresponding dual form. Now, consider the primal problem in the form of Lagrangian:

$$\begin{aligned} L = \quad & \frac{1}{2} \|X_i \omega_i^{j+1} + b_i^{j+1} e\|^2 + c e^T \xi_i^{j+1} + \\ & \alpha^T (e - \xi_i^{j+1} - e\epsilon - Z_i(\hat{X}_i \omega_i^{j+1} + b_i^{j+1} e)) + \\ & \beta^T \left(Z_i(\hat{X}_i \omega_i^{j+1} + b_i^{j+1} e) - e - \frac{\xi_i^{j+1}}{\tau} - e\frac{\epsilon}{\tau} \right) - \gamma^T (\xi_i^{j+1}), \end{aligned} \quad (10)$$

here $\alpha, \beta, \gamma \geq 0$ are the Lagrangian multiplier vectors. Now applying the KKT conditions [31], we obtain:

$$u = -(H^T H)^{-1} G^T (\beta - \alpha), \quad (11)$$

where $G = Z_i[\hat{X}_i \ e]$, $H = [X_i \ e]$, and $u = \begin{bmatrix} \omega_i^{j+1} \\ b_i^{j+1} \end{bmatrix}$.

We add a small regularization term δI , $\delta > 0$ to $H^T H$, to prevent the ill-conditioning of $H^T H$. Here I is the identity matrix of appropriate dimensions. We obtain the modified equation as:

$$u = -(H^T H + \delta I)^{-1} G^T (\beta - \alpha), \quad (12)$$

We continue to use (11) from here on wards with the understanding that if need arises (12) can be used in place of (11). Now, applying the KKT conditions, our Lagrangian is modified to give the following dual problem:

$$\begin{aligned} \min_{\alpha-\beta} \quad & \frac{1}{2}(\beta - \alpha)^T G(H^T H)^{-1} G^T (\beta - \alpha) - (\beta - \alpha)^T e + \\ & e\epsilon \left(\alpha^T + \frac{\beta^T}{\tau} \right) \\ \text{s.t.} \quad & \alpha, \beta, \gamma \geq 0, ce = \alpha + \frac{\beta}{\tau} + \gamma \end{aligned} \quad (13)$$

Making the substitution $\lambda = \alpha - \beta$. in (13) to get a simplified expression:

$$\begin{aligned} \min_{\lambda} \quad & \frac{1}{2} \lambda^T G(H^T H)^{-1} G^T \lambda - \lambda^T e \left(\frac{\epsilon}{\tau} + 1 \right) + \alpha^T e \left(\epsilon + \frac{\epsilon}{\tau} \right) \\ \text{s.t.} \quad & \alpha \geq 0, \lambda \geq 0, \alpha \left(1 + \frac{1}{\tau} \right) - \frac{\lambda}{\tau} \leq ce. \end{aligned} \quad (14)$$

After the solution of (14) is obtained, we get $[\omega_i^j; b_i^j] = -(H^T H)^{-1} G^T (\beta - \alpha)$. For the i^{th} cluster center plane, we stop after $\|[\omega_i^{j+1}; b_i^{j+1}] - [\omega_i^j; b_i^j]\| < \nu$, where ν is the error tolerance. One can also set maximum number of iterations in case the error stays above ν . For a point x_k , we can predict the label $\hat{y}(x_k) = \arg \min_{i=1,2,\dots,N} |\omega_i^T x_k + b_i|$. Here N denotes the number of clusters.

B. Non-linear SPTSVC

SPTSVC can be easily extended to non-linear case by using the kernel trick. Lets consider k kernel generated cluster center planes $K(x, X)z_i + b_i = 0$, $i = 1, \dots, k$, where $K(\cdot, \cdot)$ is an arbitrary kernel function [32], selected on the basis of the problem. Similar to the linear case, the objective function for non-linear case can be formulated as:

$$\begin{aligned} \min_{\omega_i, b_i, \xi_i, X_i} \quad & \frac{1}{2} \|K(X_i, X)z_i + b_i e\|^2 + ce^T \xi_i \\ \text{s.t.} \quad & |K(\hat{X}_i, X)z_i + b_i e| \geq e - \xi_i - e\epsilon, \\ & |K(\hat{X}_i, X)z_i + b_i e| \leq e + \frac{\xi_i}{\tau} + e\frac{\epsilon}{\tau} \\ & \xi_i \geq 0, \end{aligned} \quad (15)$$

Again, using CCCP, (15) can be reduced to smaller convex quadratic optimization problems. We obtain the following relations, which are almost identical to the linear case:

$$u = -(P^T P + \delta I)^{-1} Q^T (\beta - \alpha), \quad (16)$$

where $\delta > 0$, $Z_i = \text{diag}(\text{sign}(K(\hat{X}_i, X)z_i^j + b_i^j e))$, $P = [K(X_i, X) \ e]$, $Q = Z_i[K(\hat{X}_i, X) \ e]$, and $u = \begin{bmatrix} z_i^{j+1} \\ b_i^{j+1} \end{bmatrix}$.

In a similar manner to the linear case, the dual formulation for (15) is obtained as:

$$\begin{aligned} \min_{\alpha-\beta} \quad & \frac{1}{2}(\beta - \alpha)^T Q(P^T P)^{-1} Q^T (\beta - \alpha) - (\beta - \alpha)^T e \\ & + e\epsilon(\alpha^T + \frac{\beta^T}{\tau}) \\ \text{s.t.} \quad & \alpha, \beta, \gamma \geq 0, ce = \alpha + \frac{\beta}{\tau} + \gamma. \end{aligned} \quad (17)$$

Making the substitution $\lambda = \alpha - \beta$. in (17), to get a simplified expression:

$$\begin{aligned} \min_{\lambda} \quad & \frac{1}{2} \lambda^T Q(P^T P)^{-1} Q^T \lambda - \lambda^T e \left(\frac{\epsilon}{\tau} + 1 \right) + \alpha^T e \left(\epsilon + \frac{\epsilon}{\tau} \right) \\ \text{s.t.} \quad & \alpha \geq 0, \lambda \geq 0, \alpha \left(1 + \frac{1}{\tau} \right) - \frac{\lambda}{\tau} \leq ce. \end{aligned} \quad (18)$$

IV. DISCUSSION

In this section, we first provide rigorous analysis of noise-insensitive and sparsity properties of the proposed SPTSVC. Then, we discuss the time complexity of SPTSVC.

A. Noise insensitivity and Sparsity

The main advantage of the proposed SPTSVC model is incorporating the property of noise-insensitivity, while at the same time maintaining the sparsity of the model. The ϵ -insensitive pinball loss function $\mathcal{L}_\tau^\epsilon$ is non-differentiable at points $u = \epsilon$ and $u = -\frac{\epsilon}{\tau}$. Hence, for solving the QPP at each CCCP [30] iteration j , the sub-gradient of $\mathcal{L}_\tau^\epsilon$ is needed [33]. Sub-gradient of $\mathcal{L}_\tau^\epsilon(u)$, denoted by $g_\tau^\epsilon(u)$ is given as:

$$g_\tau^\epsilon(u) = \begin{cases} 1 & u > \epsilon, \\ [0, 1] & u = \epsilon, \\ 0 & -\frac{\epsilon}{\tau} < u < \epsilon \\ [0, 1] & u = -\frac{\epsilon}{\tau}, \\ -\tau & u < -\frac{\epsilon}{\tau}, \end{cases}$$

Further, we also partition the data-point indices j belonging to $cluster_i$ having parameters $[\omega_i; b_i]$, into 5 sets as follows:

$$\begin{aligned} S_1 &= \{j : 1 - |\omega_i^T x_j + b_i| > \epsilon\}, \\ S_2 &= \{j : 1 - |\omega_i^T x_j + b_i| = \epsilon\}, \\ S_3 &= \{j : -\frac{\epsilon}{\tau} < 1 - |\omega_i^T x_j + b_i| < \epsilon\}, \\ S_4 &= \{j : 1 - |\omega_i^T x_j + b_i| = -\frac{\epsilon}{\tau}\}, \\ S_5 &= \{j : 1 - |\omega_i^T x_j + b_i| < -\frac{\epsilon}{\tau}\}. \end{aligned}$$

Set S_5 denotes the points which are greater than $1 + \frac{\epsilon}{\tau}$ distance away from the hyper-plane $[\omega_i; b_i]$. As τ increases, the number of points in set S_5 increases. These points then contribute to the final solution, as the sub-gradient $g_\tau^\epsilon(u)$ for the same interval is non-zero. For larger values of τ , there are many points in all sets, which makes the model less sensitive to noise around the decision boundary.

Further, it can be observed that $g_\tau^\epsilon(u)$ is 0 in the interval $(-\frac{\epsilon}{\tau}, \epsilon)$. As a result, the points belonging to the set S_2 which correspond to the same interval $(-\frac{\epsilon}{\tau}, \epsilon)$, do not contribute to the final solution. This ϵ -insensitive zone leads to sparsity in the solution. This sparsity is due to the novel approach proposed in this work, which improves the drawbacks in the previous twin SVM based clustering methods.

B. Time Complexity

The solution of TWSVC requires the solutions of QPPs. For p clusters, p number of QPPs are solved for the clustering of data. Moreover, the time complexity of solving a QPP with k number of constraints is $O(k^3)$ [24]. Therefore, the total time complexity of the TWSVC algorithm is $O(pk^3)$.

On the other hand, proposed SPTSVC involves the solution of QPPs with twice the number of constraints as that in TWSVC. This is due to the ϵ -insensitive loss function in SPTSVC. Therefore, the time complexity of SPTSVC is $O(p(8k^3))$. Clearly, the computational time of proposed SPTSVC is eight times that of TWSVC. However, this can be seen as a tradeoff for the noise insensitivity of proposed SPTSVC, in comparison to existing algorithms. The computation time of calculating the inverses in SPTSVC is same as in TWSVC.

V. NUMERICAL EXPERIMENTS

This section presents the results of experiments on various clustering datasets. The proposed SPTSVC is compared with FCM [34], TWSVC [24], and TBSVC [26]. In order to test the noise-insensitivity of the proposed SPTSVC, we added zero-mean Gaussian noise to datasets with different standard deviation σ . For all the algorithms, Gaussian kernel function $K(x, y) = \exp(-\|x - y\|^2 / (2\mu^2))$ is used. All the experiments are performed using MATLAB R2017a, installed on a Windows 10 PC with 128 GB RAM, Intel(R) Xeon(R) CPU E5-2697 v4 @ 2.30GHz CPU. The codes of the proposed algorithm will be available on the author's Github page: <https://github.com/mtanveer1>.

A. Parameter selection

For the parameter selection, we used 5-fold cross-validation using the grid search method. For TWSVC, TBSVC and SPTSVC, the value of penalty parameter c is selected from the set $\{2^i | i = -5, -3, \dots, 3, 5\}$. For ϵ -insensitive pin-ball loss, the value of the parameter τ is selected from the set $\{0.25, 0.50, 1\}$ and ϵ from the set $\{0.1, 0.3, 0.5\}$. The parameter δ is taken as 10^{-4} . The value of the Gaussian kernel parameter μ is selected from the range $\{2^i | i = -5, -4, -3, \dots, 3, 4, 5\}$ for all the methods. In case of FCM, the parameter m is selected from the set $\{1, 1.25, 1.5, 1.75, 2, 2.25, 2.5\}$ [35].

B. Benchmark datasets

Experiments are performed on various benchmark datasets. The datasets include synthetic as well as real world datasets. The synthetic datasets are taken from the website: <https://github.com/deric/clustering-benchmark/tree/master/src/main/resources/datasets/artificial>. The real-world datasets are taken from the UCI Machine Learning Repository [36]. The datasets are further included with different feature noise by adding zero mean Gaussian noise with standard deviation σ set as 0 (noise-free), 0.05 and 0.1.

TABLE I: Comparison of clustering accuracy obtained on UCI and synthetic datasets with different noise levels.

Datasets (Samples $\times$ Features $\times$ Clusters)	Noise σ	FCM [34] Accuracy(%) Time (s)	TWSVC [24] Accuracy(%) Time (s)	TBSVC [26] Accuracy(%) Time (s)	SPTSVC Accuracy(%) Time (s)
ds4c2sc8 (485 $\times$ 2 $\times$ 8)	0	26.4562	95.1804	94.7466	94.6478
	0.05	0.0716	0.7969	0.5560	9.5016
	0.1	69.0206	76.7526	76.8127	77.2466
	0.1	0.1342	0.6770	0.5992	9.0470
hayes-roth (132 $\times$ 4 $\times$ 3)	0	71.2027	76.2801	77.0103	77.1735
	0.05	0.1410	0.6357	0.5588	8.8263
	0.1	60.3943	77.0462	79.1499	79.8746
	0.1	0.0119	0.0390	0.0309	0.1827
jain (373 $\times$ 2 $\times$ 2)	0	60.9778	68.939	66.0057	68.4034
	0.05	0.0122	0.0414	0.0325	0.1710
	0.1	59.8336	63.7607	63.7835	62.6279
	0.1	0.0025	0.0374	0.0351	0.1695
lense (24 $\times$ 4 $\times$ 3)	0	52.3068	100	100	100
	0.05	0.0069	0.1281	0.1177	0.6755
	0.1	51.8732	96.8152	98.9189	97.8739
	0.1	0.0036	0.1479	0.1198	0.6580
libras (360 $\times$ 90 $\times$ 15)	0	51.5449	97.9027	96.2811	97.3265
	0.05	0.0065	0.1256	0.1242	0.6551
	0.1	50	68	82	78
	0.1	0.0037	0.0210	0.0166	0.0127
lsun (400 $\times$ 2 $\times$ 3)	0	46.6667	65.3333	67.3333	74
	0.05	0.0091	0.0166	0.0142	0.0375
	0.1	60	68	66	72
	0.1	0.0012	0.0119	0.0130	0.0135
new-thyroid (215 $\times$ 5 $\times$ 3)	0	67.9734	91.4554	80.1565	91.4867
	0.05	0.6308	0.5774	0.5810	9.4616
	0.1	56.4319	88.3177	88.0047	87.9186
	0.1	0.9540	0.5194	0.5049	10.4479
seeds (210 $\times$ 7 $\times$ 3)	0	41.1189	87.9186	87.3944	87.5352
	0.05	0.0317	0.5592	0.5212	10.7237
	0.1	70.3987	100	100	99.2595
	0.1	0.0062	0.1806	0.1553	1.3830
spherical_4_3 (400 $\times$ 3 $\times$ 4)	0	70.1519	97.4241	97.5696	98.2911
	0.05	0.0225	0.1920	0.1526	1.4916
	0.1	68.7215	91.7152	91.6962	89.5759
	0.1	0.0218	0.1816	0.1466	1.4028
spherical_5_2 (250 $\times$ 2 $\times$ 5)	0	53.4219	86.4673	79.6013	89.0587
	0.05	0.0038	0.0608	0.0593	0.5206
	0.1	53.4219	89.3245	80.7752	87.309
	0.1	0.0031	0.0566	0.0554	0.5024
spherical_5_2 (250 $\times$ 2 $\times$ 5)	0	53.4219	87.4419	81.9491	85.4707
	0.05	0.0037	0.0674	0.0549	0.4823
	0.1	33.3566	85.5517	81.417	85.8537
	0.1	0.0336	0.0643	0.0493	0.3950
spherical_5_2 (250 $\times$ 2 $\times$ 5)	0	33.3566	81.8351	85.0871	82.9501
	0.05	0.0248	0.0511	0.0516	0.3951
	0.1	33.3566	73.6353	81.9512	76.3995
	0.1	0.0172	0.0539	0.0479	0.3911
tae (150 $\times$ 5 $\times$ 3)	0	95.0633	99.7658	100	99.4747
	0.05	0.0098	0.2157	0.1911	2.1070
	0.1	94.3165	100	100	98.6962
	0.1	0.0033	0.2136	0.2038	2.2116
teachingeval (151 $\times$ 5 $\times$ 3)	0	94.5759	98.8671	98.9241	100
	0.05	0.0120	0.2585	0.1945	2.1557
	0.1	78.498	96.4735	93.6816	94.9224
	0.1	0.0223	0.1289	0.1049	1.2002
tetra (400 $\times$ 3 $\times$ 4)	0	75.8041	90.6449	89.5673	90.9224
	0.05	0.0088	0.1006	0.1023	1.1128
	0.1	74.7918	85.9265	85.7796	88.2286
	0.1	0.0152	0.1221	0.0973	1.1067
zelnik1 (299 $\times$ 2 $\times$ 3)	0	32.092	62.7586	61.6092	61.5632
	0.05	0.0298	0.0301	0.0335	0.1960
	0.1	32.092	57.1034	56	57.0115
	0.1	0.0178	0.0337	0.0329	0.1963
zelnik1 (299 $\times$ 2 $\times$ 3)	0	32.092	55.8621	56.5517	56.6437
	0.05	0.0284	0.0300	0.0310	0.1944
	0.1	33.8969	60.4212	61.9726	62.9692
	0.1	0.0028	0.0323	0.0321	0.2278
zelnik1 (299 $\times$ 2 $\times$ 3)	0	33.8969	58.1001	58.3908	57.2621
	0.05	0.0189	0.0335	0.0348	0.2086
	0.1	33.8969	57.3615	56.0623	55.4127
	0.1	0.0012	0.0311	0.0334	0.1900
zelnik1 (299 $\times$ 2 $\times$ 3)	0	73.0506	100	94.8038	100
	0.05	0.0220	0.1932	0.1823	2.1000
	0.1	72.2152	98.9367	99.2025	99.2025
	0.1	0.0194	0.1922	0.1761	2.3028
zelnik1 (299 $\times$ 2 $\times$ 3)	0	71.4241	98.3038	98.5506	98.5506
	0.05	0.0203	0.1855	0.1713	2.1862
	0.1	58	99.6949	100	98.9815
	0.1	0.0420	0.1006	0.0937	0.8230
zelnik1 (299 $\times$ 2 $\times$ 3)	0	56.247	56.0374	54.9764	57.6295
	0.05	0.0175	0.1077	0.0915	0.5694
	0.1	55.4358	52.7878	55.7565	54.9784
	0.1	0.0266	0.0942	0.0920	0.7501
Average Accuracy		56.9714	82.0034	81.5589	82.6841
Average Rank		3.9048	2.0833	2.1191	1.8929
Average Training Time		0.0590	0.1749	0.1547	2.0806

TABLE II: Number of non-zero dual variables for different algorithms.

Dataset	ϵ	TWSVC	TBSVC	SPTSVC		
				$\tau = 0.25$	$\tau = 0.5$	$\tau = 1$
ds4c2sc8	0	17.4	54.375	339.45	339.425	339.5
	0.1			138.625	149.45	144.875
	0.3			73.9	90.1	88.525
	0.5			48.825	60.575	70.05
	0.5					
hayes-roth	0	28.8	40.467	70.4	70.4	70.4
	0.1			56.933	56.2	58.133
	0.3			30.4	42.2	45.6
	0.5			29.333	28.733	33.733
	0.5					
jain	0	14.9	25	149.2	149.2	149.2
	0.1			70.2	76	79.2
	0.3			39.4	47.7	52.3
	0.5			24.6	32.8	39.4
	0.5					
lense	0	5.8	5.733	12.8	12.8	12.8
	0.1			9.467	9.867	9.933
	0.3			8.533	8.533	8.6
	0.5			8.067	7.867	7.933
	0.5					
libras	0	139.32	158.347	256.48	256.547	256.84
	0.1			177.067	193.573	207.027
	0.3			142.707	150.947	160.187
	0.5			128.227	131.267	136.053
	0.5					
lsun	0	8.933	18.733	213.333	213.333	213.333
	0.1			87.867	100.133	109.733
	0.3			50.667	62.267	74.4
	0.5			29.533	39.267	49.467
	0.5					
new-thyroid	0	22.333	25.533	114.667	114.667	114.6
	0.1			58.133	53.4	61.867
	0.3			27.933	30.667	36.467
	0.5			30.533	24.933	27.067
	0.5					
seeds	0	17.067	22.933	112	112	112
	0.1			57	68.667	79.667
	0.3			31.667	36.467	43.667
	0.5			26.4	28.667	30.867
	0.5					
spherical_4_3	0	22.45	20.7	240	239.9	239.85
	0.1			48.75	55.55	59.15
	0.3			24.7	29.75	33.15
	0.5			15.5	19.8	24.45
	0.5					
spherical_5_2	0	11.04	49.88	159.96	160	159.96
	0.1			68.84	73.4	78.2
	0.3			36.08	47.28	54.48
	0.5			25.4	30.8	37.08
	0.5					
tae	0	27.4	70.533	74.333	74.4	74.4
	0.1			62.7333	64.4	66.2
	0.3			55.4	59	60.333
	0.5			51.6	51.933	52.067
	0.5					
teachingeval	0	56.467	68.6	79.733	79.533	79.4
	0.1			64.333	70.267	72.267
	0.3			48.133	54.4	59.333
	0.5			38.067	43.133	48.2
	0.5					
tetra	0	72.25	177.9	240	240	240
	0.1			129.7	164.65	187.05
	0.3			58.5	63.1	93.9
	0.5			47.55	47.55	47.55
	0.5					
zelnik1	0	20.4	72.4	158.733	158.733	158.667
	0.1			52.4	59.7333	67.533
	0.3			31.333	34.733	40.067
	0.5			26.667	28.467	30.733
	0.5					

C. Discussion on experimental results

The experimental results of the different algorithms are shown in Table I. It is observable from Table I that the proposed SPTSVC is performing better than existing algorithms in terms of clustering of the different datasets. The proposed SPTSVC achieves an average accuracy 82.68% and average rank 1.89. However, in terms of training time, the proposed SPTSVC is taking more time than the other algorithms. This is due to the ϵ -insensitive constraint in the formulation of the proposed SPTSVC, as discussed in time complexity analysis.

D. Statistical analysis

To verify the significant difference between the methods, we apply the Friedman test [37] and Nemenyi post-hoc test [37]. The Friedman test is calculated on the basis of χ^2 , using the rank of each algorithm given in Table I. Here, first we assume that all methods are having similar performance as null hypothesis. The χ^2 value is calculated to be 67.0639.

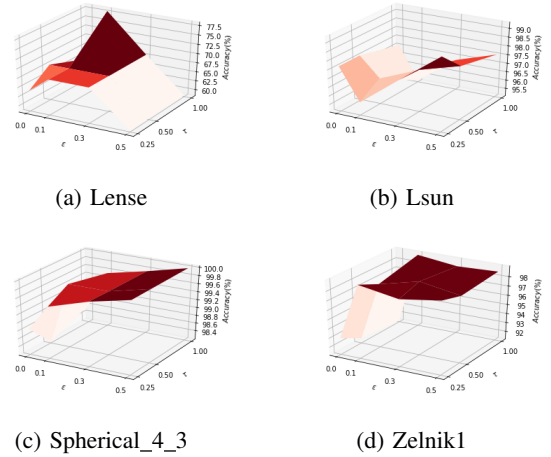


Fig. 2: 3D surface showing accuracy sensitivity of the proposed SPTSVC with respect to model parameters ϵ and τ .

$$F_F = \frac{(42 - 1) \times 67.0639}{42 \times 3 - 67.0639} \approx 46.6539. \quad (19)$$

Now, degrees of freedom for F-distribution is calculated as $(l - 1, (l - 1)(N - 1))$. For $l = 4$ and $N = 42$, the F-distribution has (3,123) degrees of freedom. For (3,123) degrees of freedom and $\alpha = 0.05$ level of significance, the critical value is 2.6783. As $F_F = 46.6539 > 2.6783$, null hypothesis does not hold true.

Further, to determine pair-wise statistical difference between algorithms, we utilize the Nemenyi post-hoc test [37].

$$CD = 2.569 \times \sqrt{\frac{4 \times 5}{6 \times 42}} \approx 0.7237. \quad (20)$$

Here, $CD = 0.7237$ denotes critical difference at $\alpha = 0.05$. Therefore, there is significant difference between the methods if difference between average ranks of the algorithms is atleast CD by the Nemenyi test [37]. So, there is significant difference between the proposed SPTSVC and FCM algorithm, but no statistical difference with TWSVC [24], and TBSVC [26].

E. Parameter Sensitivity

The 3D surface plots in Fig. 2 show the variation in accuracy with changes in parameters ϵ and τ . It can be inferred from these plots that the accuracy obtained is quite sensitive to parameters chosen. Therefore, the choice of parameters depends on the distribution of points in a particular dataset. In absence of a proper-mechanism to select optimal parameters, we have grid-searched over wide range of values for all the parameters.

F. Sparsity analysis

The sparsity is illustrated in terms of total number of non-zero dual variables in Table II. The sparseness of the proposed algorithm is shown for different values of ϵ and τ . The number of non-zero dual variables are averaged for the

different classes. The proposed SPTSVC is able to generate the clustering hyperplanes with sparsity similar to TWSVC and TBSVC. Further, It can be observed from Table II that with increase in the value of ϵ , the sparsity increases and with increase in value of τ , sparsity decreases. This is due to widening and narrowing of the ϵ -insensitive zone respectively. One more observation is more number of non-zero dual variables of TBSVC in comparison to TWSVC in Table II. This is due to the use of regularization in TBSVC algorithm.

VI. BIOMEDICAL APPLICATIONS

In this section, we illustrate the applicability of the proposed SPTSVC clustering method on biomedical time-series and image data.

A. EEG signal clustering

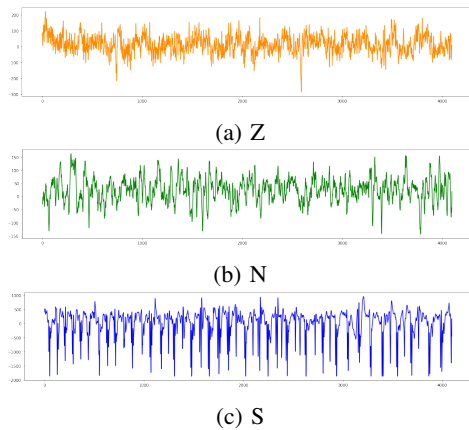


Fig. 3: Samples from EEG dataset [38].

TABLE III: EEG clustering results.

Dataset	FCM	TWSVC	TBSVC	SPTSVC
EEG	47.7253	68.4283	69.5232	71.1192

We show the clustering performance of the different algorithms on the single channel voltage recordings of EEG signals. The EEG dataset [38] utilized for this application contains five classes - Z, O, N, F and S. The classes includes one class of seizure data, and 2 classes each of healthy and seizure free signals. Some of the sample signals of the dataset are shown in Fig. 3. We applied independent component analysis (ICA) [6] to extract the prominent features for clustering of the time-series data. The results of the clustering performance of the different algorithms are shown in Table III.

B. Breast cancer clustering

TABLE IV: Breast cancer clustering results.

Dataset	FCM [34]	TWSVC [24]	TBSVC [26]	SPTSVC
BreKHis	26.4367	77.9114	78.2278	78.6772

For application on breast cancer data, we have taken the images from the BreKHis dataset [39], [7]. The dataset

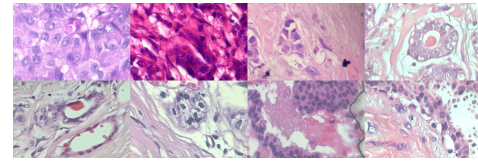


Fig. 4: Sample images from BreKHis dataset [39].

consists of 4 benign and 4 malignant types of samples. The different types of benign breast tumors are as: phyllodes tumor, fibroadenoma, adenosis, and tubular adenoma. The malignant tumors are lobular, papillary, mucinous, and ductal carcinoma. The different images from each class in the dataset are shown in Fig. 4.

We selected 50 images from each of the different classes. The features from the histopathological images are extracted using principal component analysis (PCA) method. This resulted into a dataset size of 400×100 . The comparative performance of the different algorithms on clustering of the breast cancer dataset is shown in Table IV.

C. Discussion of results on biomedical data

For EEG dataset, from the Table III, one can clearly observe the superior performance of the proposed SPTSVC model. This suggests that the proposed SPTSVC can be potentially used for the detection of EEG signals. Further, the results obtained also hint at the potential use of the proposed SPTSVC model for automated diagnosis of diseases involving EEG signals such as epilepsy. Moreover, the effectiveness of proposed model for EEG implies its usage for several applications, such as brain computer interface (BCI), detecting brain dysfunction etc.

The results obtained for breast-cancer clustering dataset has been shown in Table IV. We can infer that the proposed SPTSVC performed slightly better than the existing plane-based clustering algorithms for clustering of breast tumour images. This shows the possible applicability of proposed SPTSVC on clustering of various image datasets for biomedical applications involving MRI images, X-ray, and other multimodal imaging data.

VII. CONCLUSION AND FUTURE DIRECTIONS

In this paper, we presented a novel clustering algorithm termed as sparse pinball loss twin support vector clustering (SPTSVC). The proposed SPTSVC includes an ϵ -insensitive pinball loss function, in comparison to the traditional hinge loss. The novelty and main advantage of the proposed model is accommodating noise-insensitivity property while at the same time providing good sparsity, which leads to lesser running time. Pinball loss function also provides re-sampling stability, which is useful for large scale datasets. Thus, the proposed algorithm can be useful for various noise corrupted datasets. Further, the proposed SPTSVC gave better performance on biomedical time-series and image data.

In future, the proposed algorithm can be used in various applications involving noisy data. The proposed algorithm can be useful for applications involving less time for prediction

of labels, as testing time of proposed algorithm is lesser due to sparsity. In future, models can be developed to decrease the training time of the proposed model. In order to avoid grid-searching over wide range of parameters, there is a need to develop an efficient parameter selection methodology. For further experiments, the concept of ϵ -insensitive zone can be used with other loss functions in order to increase the sparsity while still maintaining the desired properties of the loss function in hand.

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