Quadratic Surface Support Vector Machine with L1 Norm Regularization

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Abstract

We propose \(\ell_1\) norm regularized quadratic surface support vector machine models for binary classification in supervised learning. We establish their desired theoretical properties, including the existence and uniqueness of the optimal solution, reduction to the standard SVMs over (almost) linearly separable data sets, and detection of true sparsity pattern over (almost) quadratically separable data sets if the penalty parameter of \(\ell_1\) norm is large enough. We also demonstrate their promising practical efficiency by conducting various numerical experiments on both synthetic and publicly available benchmark data sets.

Keywords. binary classification, support vector machines, quadratic support vector machines, L1 norm regularization

1 Introduction

Machine learning has recently found an extensive range of applications in various fields of contemporary science, including computer science, statistics, engineering, biology, and applied mathematics [7, 10]. Several well-received industrial applications in which machine learning has performed well are healthcare, finance, retail, travel, and media [15]. Nonetheless, compared to this significant applicability demonstrations in machine learning, rigorous theoretical studies in analyzing its models and verifying the correctness of obtained results can be improved.

Supervised learning is a major category of machine learning where labels are also available. Data classification is a vital task in supervised learning that extracts valuable information from available data, and exploits them to assign a new data point to a class [8]. Proposed by Vapnik et al. [3] and well developed in the recent twenty years, support vector machine (SVM) is an effective and efficient tool for classification. Given a labeled data set with two classes, the soft margin SVM model [3] finds a separating hyperplane with maximized margin and minimized mis-classification. It separates any (almost) linearly separable data set (almost) perfectly but fails to perform well when the data set is only nonlinearly separable.

To deal with data sets the are only nonlinearly separable, SVM models with kernel functions were proposed [3]. The idea is to use a nonlinear kernel function and map the data to (a feature space embedded into) a higher dimensional space. Then, the SVM model is applied for the classification of the mapped data in this feature space. However, for a given data set, there is no general principle
for the selection of an appropriate kernel function. Besides, the performance of kernel-based SVM models heavily depends on the parameters of a kernel function \[4, 20\]. Tuning such parameters often entails a cross-validation procedure in which parameters with maximal accuracy classification score are adopted. Therefore, training kernel-based SVM models often requires much extra computational efforts.

To take advantage of the idea of SVM while avoiding the challenges in using nonlinear kernel trick, a kernel-free quadratic surface SVM (QSSVM) model was proposed by Dagher \[5\]. Luo et al. recently developed its extension, the so called soft margin quadratic surface SVM (SQSSVM), that incorporates noise and outliers \[12\]. Both models seek a quadratic separating surface that maximizes an approximation of a relative geometric margin \[5, 12\], while the SQSSVM handles non-separable data sets by penalizing mis-classifications of outliers and noise. These models are more tractable than kernel-based SVM models because the quadratic structure of the separation surface is explicit and clear \[12\].

However, both QSSVM and SQSSVM fail to reduce to a hyperplane when a given data set is linearly separable; a natural expectation from an extension of the SVM. In addition, it is favorable to capture the possible sparsity of the hessian matrix of the separating quadratic surface especially when the number of features increases. A potential remedy to resolve these issues is adding an \(\ell_p\) norm regularization term to the objective function. There is a broad literature available on the effects of this term on the optimal solution set for different values of \(p\) in terms of uniqueness, stability, performance, and sparsity \[17, 19, 21\]. In particular, \(\ell_1\) norm regularization has demonstrated its effectiveness in machine learning and sparse optimization \[11, 16\].

To eliminate the mentioned shortcomings of QSSVM and SQSSVM models and inspired by desirable properties of \(\ell_1\) norm regularization, we propose their \(\ell_1\) norm regularized extensions, namely, L1-QSSVM and L1-SQSSVM; see Section 3. We rigorously study several interesting theoretical properties of these models, including solution existence and uniqueness, and reduction to the original SVM for (almost) linear separable data sets, and accurate sparsity pattern detection for (almost) quadratically separable data sets if the penalty parameter for the \(\ell_1\) norm regularization is large enough. To further examine our models and evaluate their numerical performance, we conduct computational experiments on both artificially generated and widely used benchmark data sets. The numerical results confirm that the proposed models outperform their parental models like the original SVM, SSVM, QSSVM, and also quadratic kernel-based model with respect to classification accuracy.

Roughly speaking, the penalty parameter for the \(\ell_1\) norm regularization not only provides various interesting properties but also controls the curvature of the separating surface from quadratic to linear a priori; such that the larger this parameter is, the more this surface resembles a line. This key property opens up a range of separating surfaces for training a data set, which is beneficial especially when a prior knowledge is available. In other words, if we speculate a data set can be separated by a linear-type surface, we can select this parameter to be relatively large, while smaller values are appropriate choices for more quadratic-type surfaces. On the contrary, the SVM, and SSVM only capture hyperplanes and QSSVM, SQSSVM only produce quadratic surfaces even if data set is linearly separable.

The rest of this paper is organized as follows. In Section 2, we bring some preliminaries that facilitate writing and reading the paper. Section 3 lays down the foundation of different models discussed and proposed in this paper. We investigate different properties of new models L1-QSSVM and L1-SQSSVM in Section 4. We conclude the paper with various numerical experiments that demonstrate the behaviour and performance of the introduced models in Section 5.

## 2 Notations and Preliminaries

In this section, we introduce some notations as well as preliminaries to be used in this paper. This section is separated into two subsections. The first subsection mainly focuses on notations and preliminaries regarding matrices, while the second focuses on convex programs.
2.1 Symmetric Matrices and Vectorization

Throughout this paper, we use lowercase letters to represent scalars, lower case bold letters to represent vectors, and uppercase bold letters to represent matrices. The set of real numbers is written as $\mathbb{R}$, and the $n$-dimensional nonnegative orthant is written as $\mathbb{R}_n^+$. We use $1_n$ to represent all one vector of length $n$, $0_{m \times n}$ to represent all 0 matrix of size $m \times n$, and $I_n$ to represent the $n \times n$ identity matrix. Let $\mathbb{S}_n$ be the set of all real symmetric $n \times n$ matrices. For $A \in \mathbb{S}_n$, we write $A \succ 0$ to denote that $A$ is positive definite and $A \succeq 0$ to denote that $A$ is positive semidefinite. For a square matrix $A = [a_{ij}]_{i=1,\ldots,n; j=1,\ldots,n} \in \mathbb{S}_n$, its vectorization is the $n^2$-vector formed by stacking up the columns of $A$, i.e., the vectorization of $A$ is given by:

$$\text{vec}(A) = [a_{11}, \ldots, a_{n1}, a_{12}, \ldots, a_{n2}, \ldots, a_{1n}, \ldots, a_{nn}]^T \in \mathbb{R}^{n^2}.$$ 

For symmetric matrix $A$, $\text{vec}(A)$ contains repeated information, since all the information is contained in the $\frac{1}{2}n(n+1)$ entries on and below the main diagonal. Therefore, we often consider half-vectorization of a symmetric matrix $A$, which is given by:

$$\text{hvec}(A) = [a_{11}, \ldots, a_{n1}, a_{22}, \ldots, a_{n2}, \ldots, a_{nn}]^T \in \mathbb{R}^{\frac{n(n+1)}{2}}.$$ 

It has been shown in [13] that, given $n$, there is a unique elimination matrix $L_n \in \mathbb{R}^{\frac{n(n+1)}{2} \times n^2}$, such that

$$L_n \text{vec}(A) = \text{hvec}(A), \quad \forall A \in \mathbb{S}_n.$$ 

For example, when $n = 3$, the elimination matrix

$$L_3 = \begin{bmatrix}
1 & 0 & 0 & 0 & 3 \\
0 & 1 & 0 & 1 & 3 \\
0 & 0 & 1 & 0 & 3 \\
0 & 0 & 1 & 1 & 3 \\
0 & 1 & 0 & 0 & 3 \\
0 & 0 & 1 & 0 & 3 \\
0 & 0 & 1 & 0 & 1 \\
0 & 0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 & 0
\end{bmatrix}.$$ 

It is known that the elimination matrix $L_n$ has full row rank [13], which is $\frac{1}{2}n(n+1)$. In reverse, for any $n$, there also exists a unique duplication matrix $D_n \in \mathbb{R}^{n^2 \times \frac{n(n+1)}{2}}$ such that

$$D_n \text{hvec}(A) = \text{vec}(A), \quad \forall A \in \mathbb{S}_n.$$ 

When $n = 3$, the duplication matrix

$$D_3 = \begin{bmatrix}
1 & 0 & 0 & 0 & 3 \\
0 & 1 & 0 & 0 & 3 \\
0 & 0 & 1 & 0 & 3 \\
0 & 0 & 1 & 1 & 3 \\
0 & 1 & 0 & 0 & 3 \\
0 & 0 & 1 & 0 & 3 \\
0 & 0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 & 0
\end{bmatrix}.$$ 

It is also known that $D_n$ has full column rank, which is $\frac{1}{2}n(n+1)$. Moreover,

$$L_n D_n = \mathbb{I}_{\frac{n(n+1)}{2}},$$

the $\frac{n(n+1)}{2} \times \frac{n(n+1)}{2}$ identity matrix. Given two matrices $A \in \mathbb{R}^{m \times n}$ and $B \in \mathbb{R}^{p \times q}$, the Kronecker product of them is written as

$$A \otimes B = \begin{bmatrix}
a_{11}B & \cdots & a_{1n}B \\
\vdots & \ddots & \vdots \\
a_{m1}B & \cdots & a_{mn}B
\end{bmatrix} \in \mathbb{R}^{mp \times nq}.$$
Let a symmetric matrix $M$ be partitioned as follows

$$M = \begin{bmatrix} A & B \\ B^T & C \end{bmatrix}.$$  \hspace{1cm} (1)

We state the following standard lemma regarding the positive definiteness of partitioned matrix $M$.

**Lemma 2.1.** Let matrix $M$ be partitioned as (1). Then, $M$ is positive definite if and only if $C$ is positive definite and $A - BC^{-1}B^T$ is positive definite.

### 2.2 Convex Optimization and Some Standard Results

The SVM-type problems are typically modeled as convex optimization problems. We review a few related results from optimization theory in this subsection. We first consider the following quadratic program (QP):

$$\begin{aligned}
\min & \quad \frac{1}{2}x^TQx + b^Tx \\
\text{s.t.} & \quad Ax \geq c
\end{aligned} \hspace{1cm} (2)$$

where $Q \in S_p$ is a given symmetric matrix, $b \in \mathbb{R}^p$ and $c \in \mathbb{R}^q$ are given vectors, and $A \in \mathbb{R}^{q \times p}$ is a given matrix. We first provide a result regarding solution existence of the QP (2).

**Lemma 2.2.** Consider QP (2). If the objective function is bounded from below over a nonempty feasible domain, then it has a solution.

Detailed proofs of Lemma 2.2 can be found in [9] and hence is omitted here.

Our proposed optimization models in this paper are convex and comprise $\ell_1$ norm in their objective functions. Since $\ell_1$ norm is not differentiable everywhere, we present some concepts and results regarding non-smooth convex optimization problems. For a function $f(x) : \mathbb{R}^n \mapsto \mathbb{R}$, the subdifferential of it at $x$, denoted by $\partial f|_x$ is defined as

$$\partial f|_x \triangleq \{ g \in \mathbb{R}^n \mid g^T(y - x) \leq f(y) - f(x), \forall y \}.$$  

It is known that $\partial f(x)$ is a closed convex set (possibly empty) in general. But this set is nonempty and bounded for an interior point $x$ in the domain of a convex function. We are particularly interested in $\ell_1$ norm as a function for which we have

$$\partial(\|\cdot\|_1)|_x = J_1 \times J_2 \times \cdots \times J_n,$$

with

$$J_k = \begin{cases} [-1, 1] & \text{if } x_k = 0, \\
\{1\} & \text{if } x_k > 0, \\
\{-1\} & \text{if } x_k < 0. \end{cases}$$

Consider a convex optimization problem with possibly a non-smooth objective function as follows:

$$\begin{aligned}
\min & \quad f(x) \\
\text{s.t} & \quad g_i(x) \geq 0, \quad i = 1, \ldots, m.
\end{aligned}$$

Assuming that some certain constraint qualification holds at a feasible vector $x^*$, this vector is a local optimal solution of this problem if and only we have

$$0 \in \partial f(x^*) - \sum_{i=1}^{m} \alpha_i \nabla g_i(x^*),$$ \hspace{1cm} (3)

for $\alpha \in \mathbb{R}^m$ such that $\alpha_i g_i(x^*) = 0, \ i = 1, \ldots, m$; see Proposition 3.2.3, Theorem 6.1.8 and Exercise 5 of Section 7.2 in [2]. The constraint qualification of interest in our discussion is the existence of an interior feasible point for the constraints. This is guaranteed based on linear or quadratic separability assumptions depending on the situation.
3 Quadratic Surface Support Vector Machines

In this section, we introduce quadratic surface support vector machines (QSSVMs). We first describe the training data set and then discuss existing optimization models for QSSVMs. In the last subsection, we propose an $\ell_1$ norm regularized version of QSSVMs.

3.1 Training Data Set

For any classification problems, the training set is typically composed of $m$ samples each represented by a vector in $\mathbb{R}^n$ and a label. Mathematically, a training data set with two classes can be denoted by

$$
\mathcal{D} = \left\{ (\mathbf{x}^{(i)}, y^{(i)}) \right\}_{i=1,\ldots,m} \quad | \mathbf{x}^{(i)} \in \mathbb{R}^n, y^{(i)} \in \{-1,1\} \right\},
$$

where $m$ is the sample size, $n$ is the number of features, $\mathbf{x}^{(i)} = [x_1^{(i)}, \ldots, x_n^{(i)}]^T \in \mathbb{R}^n$ is the vector of feature values for sample $i$, and $y^{(i)}$ is the label for sample $i$. We let $\mathcal{M}^+ \triangleq \{i \mid y^{(i)} = 1\}$ and $\mathcal{M}^- \triangleq \{i \mid y^{(i)} = -1\}$. We assume that $\mathcal{M}^+ \neq \emptyset$ and $\mathcal{M}^- \neq \emptyset$. With the given training data, a recent approach proposed by Dagher [5] and developed by Luo et al. [12] aims to separate the data using a quadratic function:

$$
f(x) = \frac{1}{2}\mathbf{x}^T \mathbf{W} \mathbf{x} + \mathbf{b}^T \mathbf{x} + c,
$$

with $\mathbf{W} \in \mathbb{S}_n, \mathbf{b} \in \mathbb{R}^n$, and $c \in \mathbb{R}$. To facilitate the presentation, we define a few matrices and vectors. Define the sample matrix as:

$$
\mathbf{X} = \begin{bmatrix} (\mathbf{x}^{(1)})^T \\ \vdots \\ (\mathbf{x}^{(m)})^T \end{bmatrix} \in \mathbb{R}^{m \times n}.
$$

For the sake of analysis, we assume that:

(A1) $\mathbf{X}$ has full column rank.

Note that assumption (A1) is a very mild assumption. First of all, we typically have $m \gg n$. Secondly, if (A1) does not hold, then there is redundancy in the set of features. We typically remove the redundancy by conducting principle component analysis.

We say a data set $\mathcal{D}$ is quadratically separable [12] if there exists $\mathbf{W} \in \mathbb{R}^{n \times n}, \mathbf{b} \in \mathbb{R}^n, c \in \mathbb{R}$ such that

$$
\begin{align*}
\frac{1}{2}\mathbf{x}^{(i)T} \mathbf{W} \mathbf{x}^{(i)} + \mathbf{b}^T \mathbf{x}^{(i)} + c &> 0, \quad \forall i \in \mathcal{M}^+, \\
\frac{1}{2}\mathbf{x}^{(i)T} \mathbf{W} \mathbf{x}^{(i)} + \mathbf{b}^T \mathbf{x}^{(i)} + c &< 0, \quad \forall i \in \mathcal{M}^-.
\end{align*}
$$

We say a data set $\mathcal{D}$ is linearly separable [6] if there exists $\mathbf{b} \in \mathbb{R}^n, c \in \mathbb{R}$ such that

$$
\begin{align*}
\mathbf{b}^T \mathbf{x}^{(i)} + c &> 0, \quad \forall i \in \mathcal{M}^+, \\
\mathbf{b}^T \mathbf{x}^{(i)} + c &< 0, \quad \forall i \in \mathcal{M}^-.
\end{align*}
$$

Note that a linearly data set is simply quadratically separable with $\mathbf{W} = \mathbf{0}$. To develop optimization models, we introduce the following definitions.

Definition 3.1 (Vector $\mathbf{s}$ and $\mathbf{r}$). For all $i = 1, \ldots, m$, define $s^{(i)} \in \mathbb{R}^{\frac{n(n+1)}{2}}$ as

$$
s^{(i)} = \begin{bmatrix} \frac{1}{2}x_1^{(i)} x_1^{(i)} , x_1^{(i)} x_2^{(i)} , \ldots , x_1^{(i)} x_n^{(i)} , \frac{1}{2}x_2^{(i)} x_2^{(i)} , x_2^{(i)} x_3^{(i)} , \ldots , x_2^{(i)} x_n^{(i)} , \ldots , \frac{1}{2}x_n^{(i)} x_n^{(i)} \end{bmatrix}^T,
$$

and

$$
r^{(i)} = \begin{bmatrix} s^{(i)} \\ x^{(i)} \end{bmatrix}.
$$
For convenience, denote \( w = \text{hvec}(W) \) for future use.

**Definition 3.2** (Vectorized parameters \( \mathbf{z} \)). Define \( \mathbf{z} \in \mathbb{R}^{n(n+1)/2+n} \) as \( \mathbf{z} = \begin{bmatrix} \mathbf{w} \\ \mathbf{b} \end{bmatrix} \).

Hence, by definitions 3.2 and 3.1 we have

\[
\frac{1}{2} \mathbf{x}^{(i)^T} W \mathbf{x}^{(i)} + \mathbf{x}^{(i)^T} \mathbf{b} + c = \mathbf{z}^T \mathbf{r}^{(i)} + c.
\]

Let \( \mathbf{V} := \begin{bmatrix} \mathbf{I}_{n(n+1)/2} & 0_{n(n+1)/2 \times n} \end{bmatrix} \). This implies that \( \text{hvec}(W) = w = \mathbf{V} \mathbf{z} \).

**Definition 3.3.** For all \( i = 1, \ldots, m \), define \( \mathbf{X}^{(i)} \in \mathbb{R}^{n \times n^2} \) as

\[
\mathbf{X}^{(i)} = \mathbf{I}_n \otimes (\mathbf{x}^{(i)})^T = \begin{bmatrix} (\mathbf{x}^{(i)})^T \\ \vdots \\ (\mathbf{x}^{(i)})^T \end{bmatrix}.
\]

**Definition 3.4** (Matrix \( \mathbf{M}^{(i)} \)). For all \( i = 1, \ldots, m \), define \( \mathbf{M}^{(i)} \in \mathbb{R}^{n \times n(n+1)/2} \) as \( \mathbf{M}^{(i)} = \mathbf{X}^{(i)} \mathbf{D}_n \).

**Definition 3.5** (Matrix \( \mathbf{H}^{(i)} \)). For all \( i = 1, \ldots, m \), define \( \mathbf{H}^{(i)} \in \mathbb{R}^{n \times n(n+3)/2} \) as \( \mathbf{H}^{(i)} = \begin{bmatrix} \mathbf{M}^{(i)} & \mathbf{I}_n \end{bmatrix} \).

According to the above definitions, we have

\[
W \mathbf{x}^{(i)} = \mathbf{X}^{(i)^{\text{vec}}}(W) = \mathbf{X}^{(i)} \mathbf{D}_n \text{hvec}(W) = \mathbf{M}^{(i)} \text{hvec}(W) = \mathbf{M}^{(i)} w,
\]

and thus:

\[
W \mathbf{x}^{(i)} + \mathbf{b} = \mathbf{M}^{(i)} w + \mathbf{I}_n \mathbf{b} = \mathbf{H}^{(i)} \mathbf{z}.
\]

It follows that:

\[
\sum_{i=1}^{m} \left\| W \mathbf{x}^{(i)} + \mathbf{b} \right\|_2^2 = \sum_{i=1}^{m} \left( \mathbf{H}^{(i)} \mathbf{z} \right)^T \mathbf{H}^{(i)} \mathbf{z} = \mathbf{z}^T \left[ \sum_{i=1}^{m} \left( \mathbf{H}^{(i)} \right)^T \mathbf{H}^{(i)} \right] \mathbf{z}.
\]

Define

\[
\mathbf{G} := 2 \sum_{i=1}^{m} \left( \mathbf{H}^{(i)} \right)^T \mathbf{H}^{(i)},
\]

and it implies that

\[
\sum_{i=1}^{m} \left\| W \mathbf{x}^{(i)} + \mathbf{b} \right\|_2^2 = \frac{1}{2} \mathbf{z}^T \mathbf{G} \mathbf{z}.
\]

Clearly, we know that \( \mathbf{G} \succeq 0 \). We will provide conditions under which \( \mathbf{G} \succ 0 \) in a later section.

### 3.2 Quadratic Surface SVM Models

Mathematical computations for the margin of quadratic surface support vector machine suggest the following formulation:

\[
\min_{W, b, c} \sum_{i=1}^{m} \left\| W \mathbf{x}^{(i)} + \mathbf{b} \right\|_2^2
\]

\[\text{s.t.} \quad y^{(i)} \left( \frac{1}{2} \mathbf{x}^{(i)^T} W \mathbf{x}^{(i)} + \mathbf{x}^{(i)^T} \mathbf{b} + c \right) \geq 1, \quad i = 1, \ldots, m, \quad W \in \mathbb{S}_n, b \in \mathbb{R}^n, c \in \mathbb{R}. \quad (\text{QSSVM})\]

\(6\)
To compromise with possible noise and outliers in the data, the following soft margin version of QSSVM penalizes mis-classifications:

$$\min_{W, b, c, \xi} \sum_{i=1}^{m} \|Wx^{(i)} + b\|^2_2 + \mu \sum_{i=1}^{m} \xi_i$$

subject to:

$$y^{(i)} \left( \frac{1}{2} x^{(i)^T} W x^{(i)} + x^{(i)^T} b + c \right) \geq 1 - \xi_i, \quad i = 1, \ldots, m,$$

$$W \in \mathbb{S}_n, \ b \in \mathbb{R}^n, \ c \in \mathbb{R}, \ \xi \in \mathbb{R}_+^m.$$

With the notations defined in Subsection 3.1, we have the following equivalent formulation for QSSVM:

$$\min_{z, c} \frac{1}{2} z^T G z$$

subject to:

$$y^{(i)} \left( z^T r^{(i)} + c \right) \geq 1, \quad i = 1, \ldots, m,$$

$$z \in \mathbb{R}^{\frac{n(n+1)}{2} + n}, \ c \in \mathbb{R},$$

and similarly for SQSSVM:

$$\min_{z, c, \xi} \frac{1}{2} z^T G z + \mu \sum_{i=1}^{m} \xi_i$$

subject to:

$$y^{(i)} \left( z^T r^{(i)} + c \right) \geq 1 - \xi_i, \quad i = 1, \ldots, m,$$

$$z \in \mathbb{R}^{\frac{n(n+1)}{2} + n}, \ c \in \mathbb{R}, \ \xi \in \mathbb{R}_+^m.$$

### 3.3 ℓ\(_1\) Norm Regularized Quadratic Surface SVM Models

As we can see, by using quadratic surface to separate the data, the classification model complexity is increased significantly. While the complexity provides extra flexibility to separate data in the training set, it could also lead to over-fitting issues and hence inferior classification performance on testing data sets. One particular situation is when the training data set is linearly separable, it is desirable that QSSVMs can find a hyperplane to separate the data. However, there is no guarantee if we use models (QSSVM) or (SQSSVM). On the other hand, ℓ\(_1\) norm regularization technique has been shown to reduce model complexity in many application. Therefore, we propose to introduce L1-regularization into QSSVMs:

$$\min_{W, b, c} \sum_{i=1}^{m} \|Wx^{(i)} + b\|^2_2 + \lambda \sum_{1 \leq i \leq j \leq n} |W_{ij}|$$

subject to:

$$y^{(i)} \left( \frac{1}{2} x^{(i)^T} W x^{(i)} + x^{(i)^T} b + c \right) \geq 1, \quad i = 1, \ldots, m,$$

$$W \in \mathbb{S}_n, \ b \in \mathbb{R}^n, \ c \in \mathbb{R},$$

where \(\lambda\) is a positive constant that penalizes nonzero elements of the model matrix \(W\). This is equivalent to:

$$\min_{z, c} \frac{1}{2} z^T G z + \lambda \|Vz\|_1$$

subject to:

$$y^{(i)} \left( z^T r^{(i)} + c \right) \geq 1, \quad i = 1, \ldots, m,$$

$$z \in \mathbb{R}^{\frac{n(n+1)}{2} + n}, \ c \in \mathbb{R},$$
To account for outliers, we consider the following soft version of L1-QSSVM:

$$\min_{W,b,c,\xi} \sum_{i=1}^{m} \|Wx^{(i)} + b\|_2^2 + \lambda \sum_{1 \leq i \neq j \leq n} |W_{ij}| + \mu \sum_{i=1}^{m} \xi_i$$

$$s.t. \quad y^{(i)} \left( \frac{1}{2} x^{(i)^T} W x^{(i)} + x^{(i)^T} b + c \right) \geq 1 - \xi_i, \quad i = 1, \ldots, m,$$

$$W \in S_n, \ b \in \mathbb{R}^n, \ c \in \mathbb{R}, \ \xi \in \mathbb{R}_+^m,$$

where $\mu > 0$ is a positive penalty for incorporating noise and outliers. This problem can be equivalently rewritten as the following convex program:

$$\min_{z,c,\xi} \frac{1}{2} z^T G z + \lambda \|Vz\|_1 + \mu \sum_{i=1}^{m} \xi_i$$

$$s.t. \quad y^{(i)} \left( z^T r^{(i)} + c \right) \geq 1 - \xi_i, \quad i = 1, \ldots, m,$$

$$z \in \mathbb{R}^{n(n+1)/2}, \ c \in \mathbb{R}, \ \xi \in \mathbb{R}_+^m.$$

In the next section, we study theoretical properties of the proposed models.

4 Theoretical Properties of $\ell_1$ Norm Regularized QSSVMs

In this section, we explore theoretical properties of the proposed $\ell_1$ norm regularized QSSVM models. We first discuss the solution existence and uniqueness of our proposed models. We then study the soft margin models, and show that the margin vanishes when $\mu$ is large enough and the data is separable. Lastly, we examine the effects of the $\ell_1$ norm regularization.

4.1 Solution Existence and Uniqueness

**Theorem 4.1 (Solution Existence).** Given any data set $D$ defined in (4), the model L1-SQSSVM obtains an optimal solution with a finite objective value. A similar result holds for (L1-QSSVM) on any linearly or quadratically separable data set.

**Proof.** The model (L1-SQSSVM) is equivalent to (L1-SQSSVM'), which reduces to a convex quadratic program with linear constraints by a standard technique. Given a data set $D$, the feasible set is nonempty for an arbitrary $z$ and $c$ with

$$\xi_i = \max \left[ 0, 1 - y^{(i)} \left( z^T r^{(i)} + c \right) \right], \quad i = 1, \ldots, m.$$  

Further, the objective function in (L1-SQSSVM') is bounded below by zero over the feasible set. Hence, Lemma 2.2 implies that (L1-SQSSVM') has an optimal solution with a finite objective value and so as (L1-SQSSVM'). The same idea applies to the model (L1-QSSVM'). A similar argument can be applied to the second statement of the theorem.  

We next show that if $G$ is positive definite, then $z^*$ must be unique. One can prove this using tedious rewriting of (L1-SQSSVM') as a standard quadratic program and then exploiting gradient uniqueness, nonetheless we provide a direct proof below.

**Theorem 4.2 (z-Uniqueness).** Assume that the matrix $G$ defined in (8) is positive definite. Then, the solution $z^*$ is unique for the model (L1-SQSSVM').

**Proof.** Assume that $(z^*,c^*,\xi^*)$ and $(z^{**},c^{**},\xi^{**})$ are two optima of (L1-SQSSVM') such that $z^* \neq z^{**}$. Since this problem is convex, its optimal solution set is convex. Thus, any convex combination of $(z^*,c^*,\xi^*)$ and $(z^{**},c^{**},\xi^{**})$ obtains the same optimal value. Let

$$g(z,\xi) := \frac{1}{2} z^T G z + \lambda \|Vz\|_1 + \mu \sum_{i=1}^{m} \xi_i.$$  

Thus, for \( \delta \in (0, 1) \), we have

\[
q(\delta z^* + (1 - \delta)z^{**}, \delta \xi^* + (1 - \delta)\xi^{**}) = \delta q(z^*, \xi^*) + (1 - \delta)q(z^{**}, \xi^{**}).
\]

Equivalently, we have:

\[
\frac{1}{2}(\delta z^* + (1 - \delta)z^{**})^T G(\delta z^* + (1 - \delta)z^{**}) + \lambda \|\delta Vz^* + (1 - \delta)Vz^{**}\|_1 + \mu \sum_{i=1}^m (\delta \xi_i^* + (1 - \delta)\xi_i^{**})
\]

\[
= \frac{\delta}{2} z^{**T} Gz^* + \lambda \|\delta Vz^* + (1 - \delta)Vz^{**}\|_1 + \mu \sum_{i=1}^m (\delta \xi_i^* + (1 - \delta)\xi_i^{**}).
\]

Simple calculations lead to

\[
\frac{\delta^2 - \delta}{2} \left[ z^{**T} Gz^* - 2z^{**T} Gz^{**} + z^{**T} Gz^{**} \right] + \lambda \left[\|\delta Vz^* + (1 - \delta)Vz^{**}\|_1 - \|\delta Vz^*\|_1 - (1 - \delta)\|Vz^{**}\|_1 \right] = 0,
\]

which further means that

\[
\frac{\delta^2 - \delta^2}{2} \left[ (z^* - z^{**})^T G(z^* - z^{**}) \right] + \lambda \left[\|\delta Vz^* + (1 - \delta)Vz^{**}\|_1 - \|\delta Vz^*\|_1 - (1 - \delta)\|Vz^{**}\|_1 \right] = 0.
\]

Since \( \delta \in (0, 1) \) and \( \lambda > 0 \), the positive definiteness of \( G \) along with the Cauchy-Schwartz inequality imply that \( (z^* - z^{**})^T G(z^* - z^{**}) = 0 \) and \( \|\delta Vz^* + (1 - \delta)Vz^{**}\|_1 - \|\delta Vz^*\|_1 - (1 - \delta)\|Vz^{**}\|_1 = 0 \). The former equation yields \( z^* = z^{**} \).

We therefore investigate the conditions under which the matrix \( G \) is positive definite below.

**Theorem 4.3** (Positive-Definiteness of \( G \)). Let (A1) hold. Also, assume that

(A2) \( 1_m \) is not in the column space of \( X \).

Then, the matrix \( G \) defined in (8) is positive definite.

**Proof.** By the definition of \( M^{(i)} \), for all \( i = 1, \ldots, m \), we have:

\[
\begin{pmatrix} H^{(i)} \end{pmatrix}^T H^{(i)} = \begin{bmatrix} (M^{(i)})^T & M^{(i)} \\ I_n & I_n \end{bmatrix} = \begin{bmatrix} (M^{(i)})^T & \vdots \\ M^{(i)} & I_n \end{bmatrix}.
\]

Therefore,

\[
G = 2 \sum_{i=1}^m \begin{pmatrix} H^{(i)} \end{pmatrix}^T H^{(i)} = 2 \begin{bmatrix} \sum_{i=1}^m (M^{(i)})^T M^{(i)} & \vdots \\ \sum_{i=1}^m M^{(i)} & \sum_{i=1}^m M^{(i)} \end{bmatrix}.
\]  

(8)

By Lemma 2.1, it is clear that \( G \succ 0 \) if and only if

\[
\sum_{i=1}^m (M^{(i)})^T M^{(i)} - \frac{1}{m} \left( \sum_{i=1}^m M^{(i)} \right) \succ 0.
\]

By definitions, we have

\[
\sum_{i=1}^m (M^{(i)})^T M^{(i)} = \sum_{i=1}^m \left( X^{(i)} D_n \right)^T \left( X^{(i)} D_n \right) = D_n^T \left[ \sum_{i=1}^m \left( X^{(i)} \right)^T X^{(i)} \right] D_n.
\]

Similarly, we have

\[
\left( \sum_{i=1}^m M^{(i)} \right)^T \sum_{i=1}^m M^{(i)} = D_n^T \left[ \sum_{i=1}^m \left( X^{(i)} \right)^T X^{(i)} \right] D_n.
\]

\[
= D_n^T \left[ \sum_{i=1}^m \left( X^{(i)} \right)^T \left( \sum_{i=1}^m X^{(i)} \right) \right] D_n.
\]

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Since $D_n$ has full column rank, therefore
\[
G > 0 \iff D_n^T \left[ \sum_{i=1}^m (X^{(i)})^T X^{(i)} - \frac{1}{m} \left( \sum_{i=1}^m X^{(i)} \right)^T \left( \sum_{i=1}^m X^{(i)} \right) \right] D_n > 0
\]
\[
\iff \sum_{i=1}^m (X^{(i)})^T X^{(i)} - \frac{1}{m} \left( \sum_{i=1}^m X^{(i)} \right)^T \left( \sum_{i=1}^m X^{(i)} \right) > 0.
\]
For any given vector $v \in \mathbb{R}^{n^2}$, we partition $v$ into $n$ parts with equal length, i.e.,
\[
v = [(v^1)^T, (v^2)^T, \ldots, (v^n)^T]^T.
\]
We have, for each $i = 1, \ldots, n$
\[
X^{(i)} v = \begin{bmatrix} (x^{(i)})^T \\ \vdots \\ (x^{(i)})^T \end{bmatrix} \begin{bmatrix} v^1 \\ \vdots \\ v^n \end{bmatrix} = \begin{bmatrix} (x^{(i)})^T v^1 \\ \vdots \\ (x^{(i)})^T v^n \end{bmatrix}.
\]
Let $b_{ij} = (x^{(i)})^T v^j$ and $b^i = [b_{i1}, \ldots, b_{in}]^T \in \mathbb{R}^n$. We can see that $X^{(i)} v = b^i$ and hence
\[
v^T \left[ \sum_{i=1}^m (X^{(i)})^T X^{(i)} \right] v = \sum_{i=1}^m v^T (X^{(i)})^T X^{(i)} v = \sum_{i=1}^m \|b^i\|_2^2.
\]
Also, we have
\[
v^T \left[ \left( \sum_{i=1}^m X^{(i)} \right)^T \left( \sum_{i=1}^m X^{(i)} \right) \right] v = \left( \sum_{i=1}^m X^{(i)} v \right)^T \left( \sum_{i=1}^m X^{(i)} v \right)
\]
\[
\quad = \left( \sum_{i=1}^m b^i \right)^T \left( \sum_{i=1}^m b^i \right) = \left\| \sum_{i=1}^m b^i \right\|_2^2
\]
\[
\quad = \sum_{i=1}^m \|b^i\|_2^2 + \sum_{i \neq k} (b^i)^T b^k \leq \sum_{i=1}^m \|b^i\|_2^2 + \sum_{i \neq k} \|b^i\|_2 \|b^k\|_2
\]
\[
\quad \leq \sum_{i=1}^m \|b^i\|_2^2 + \sum_{i \neq k} \frac{1}{2} (\|b^i\|_2^2 + \|b^k\|_2^2) = m \sum_{i=1}^m \|b^i\|_2^2,
\]  \hspace{1cm} (9)
where the equality holds if and only if $b^1 = b^2 = \cdots = b^m$. This is equivalent to
\[
(x^{(1)})^T v^j = (x^{(2)})^T v^j = \cdots = (x^{(m)})^T v^j, \quad j = 1, \ldots, n.
\]
Since $X$ has full column rank, this in turn implies that there exists $u \in \mathbb{R}^n$ such that $X u = 1_m$. However, by assumption $1_m$ is not in the column space of $X$, therefore the inequality in (9) holds strictly. That is,
\[
v^T \left[ \sum_{i=1}^m (X^{(i)})^T X^{(i)} - \frac{1}{m} \left( \sum_{i=1}^m X^{(i)} \right)^T \left( \sum_{i=1}^m X^{(i)} \right) \right] v > 0,
\]
for all $v \in \mathbb{R}^{n^2}$ and $v \neq 0$, i.e.,
\[
\sum_{i=1}^m (X^{(i)})^T X^{(i)} - \frac{1}{m} \left( \sum_{i=1}^m X^{(i)} \right)^T \left( \sum_{i=1}^m X^{(i)} \right) > 0.
\]
This concludes the proof.
We next show that the set of $X$’s for which the associated matrix $G$ is not positive definite is of Lebesgue measure zero in $\mathbb{R}^{m \times n}$. To be more specific, we define the following set:

$$S \triangleq \{ X \in \mathbb{R}^{m \times n} \mid G \text{ is positive definite} \}. \quad (10)$$

**Theorem 4.4.** Let $m \geq n + 1$. The complement of $S$ defined in Equation (10) is of Lebesgue measure zero in $\mathbb{R}^{m \times n}$.

**Proof.** From Theorem 4.3, it suffices to show that the data matrices $X$ not satisfying assumptions (A1) or (A2) is of Lebesgue measure zero in $\mathbb{R}^{m \times n}$. We augment $X$ by appending an all 1 column to it. That is, we consider

$$X = \begin{bmatrix} X \mid 1_m \end{bmatrix}.$$

It is clear that assumptions (A1) and (A2) holds if and only if $X$ has full column rank. We let

$$S \triangleq \{ X \in \mathbb{R}^{m \times n} \mid X \text{ has linearly independent columns} \}.$$

Let $I$ be an arbitrary subset of $\{1, \cdots, m\}$ with $n + 1$ elements. Define the following polynomial:

$$\varphi_I(X) \triangleq \det(\overline{X}_I) \left( \sum_{i \notin J} \sum_{j = 1}^{n+1} [(\overline{X}_{ij})^2 + 1] \right),$$

where $\overline{X}_I$ is the submatrix formed by taking the rows with the index in $I$ of $X$. It is clear that $\varphi_I(X) = 0$ if and only if $\det(\overline{X}_I) = 0$. Let the zero set of $\varphi_I(X)$ be denoted by $z(\varphi_I(X))$. It is clear that this zero set is of Lebesgue measure 0 in $\mathbb{R}^{m \times n}$. Let the collection of all subset of $\{1, \cdots, m\}$ with $n + 1$ elements be denoted by $\Theta$. We notice that the complement of $S$ in $\mathbb{R}^{m \times n}$ is

$$S^c = \{ X \in \mathbb{R}^{m \times n} \mid \forall J \in \Theta \text{ it holds that } \det(\overline{X}_J) = 0 \}.$$

Thus,

$$S^c \subseteq \bigcap_{J \in \Theta} z(\varphi_J(X)).$$

Since the right-hand side is a finite intersection of measure zero sets, it is still a measure zero set. Therefore $S^c$ is a measure zero set in $\mathbb{R}^{m \times n}$. This concludes the proof.

While the uniqueness of $c^*$ and $\xi^*$ in L1-SQSSVM’ is in general not guaranteed, we have the following observation. Let $(z^*, \xi^*, c^*)$ be an optimal solution of (L1-SQSSVM’), it is clear that when $z^*$ is given, $(c^*, \xi^*)$ must solve the following linear program.

$$\begin{aligned}
(c^*, \xi^*) &\in \arg\min_{c, \xi} \sum_{i=1}^{m} \xi_i \\
&\text{s.t. } y^{(i)} (f_i + c) \geq 1 - \xi_i, \quad i = 1, \ldots, m, \\
&c \in \mathbb{R}, \xi \in \mathbb{R}_+^m,
\end{aligned} \quad (11)$$

where $f_i = (z^*)^T r^{(i)}$. The uniqueness of $c^*$ and $\xi^*$ is therefore related to the solution uniqueness of linear program (11). The readers can refer to [14], for results regarding solution uniqueness of linear programs. Nonetheless, we next provide some conditions under which the solution of L1-SQSSVM is unique.

### 4.2 Vanishing Margin $\xi$ in Quadratically Separable Case

As we mentioned, the training data may contain noise, and hence not separable. We include soft margin $\xi$ to handle this situation. In principle, when the data is separable, the soft margin should vanish in the solutions. In this subsection, we show that $\xi$ does vanish when the data is quadratically

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separable, if $\mu$ is large enough. For convenience, we consider the following equivalent formulations for (L1-QSSVM) and (L1-SQSSVM).

\[
\begin{align*}
\min_{w, b, c} & \quad q(w, b, c) \triangleq \sum_{i=1}^{m} w^T M^{(i)} M^{(i)} w + 2 \sum_{i=1}^{m} w^T M^{(i)} b + m b^T b + \lambda \|w\|_1 \\
\text{s.t.} & \quad y^{(i)} \left( w^T s^{(i)} + b^T x^{(i)} + c \right) \geq 1, \quad i = 1, \ldots, m, \\
& \quad w \in \mathbb{R}^{\frac{n(n+1)}{2}}, \ b \in \mathbb{R}^n, \ c \in \mathbb{R}.
\end{align*}
\] (L1-QSSVM')

\[
\begin{align*}
\min_{w, b, c, \xi} & \quad \sum_{i=1}^{m} w^T M^{(i)} M^{(i)} w + 2 \sum_{i=1}^{m} w^T M^{(i)} b + m b^T b + \lambda \|w\|_1 + \mu \sum_{i=1}^{m} \xi_i \\
\text{s.t.} & \quad y^{(i)} \left( w^T s^{(i)} + b^T x^{(i)} + c \right) \geq 1 - \xi_i, \quad i = 1, \ldots, m, \\
& \quad w \in \mathbb{R}^{\frac{n(n+1)}{2}}, \ b \in \mathbb{R}^n, \ c \in \mathbb{R}, \ \xi \in \mathbb{R}^m_+.
\end{align*}
\] (L1-SQSSVM')

It is clear that when the training data is quadratically separable, the hard margin model (L1-QSSVM') is feasible and has an optimal solution $(w^*, b^*, c^*)$. Therefore, according to (3), there exists a multiplier vector $\alpha^* \in \mathbb{R}^m$ so that $(w^*, b^*, c^*, \alpha^*)$ satisfies the following KKT conditions:

\[
\begin{align*}
& 0 \in 2 \sum_{i=1}^{m} M^{(i)} M^{(i)} w^* + 2 \sum_{i=1}^{m} M^{(i)} b^* + \lambda \partial (\|\cdot\|_1)|_{w^*} - \sum_{i=1}^{m} \alpha_i^* y^{(i)} s^{(i)}, \\
& 2 \sum_{i=1}^{m} M^{(i)} w^* + 2 m b^* = \sum_{i=1}^{m} \alpha_i^* y^{(i)} x^{(i)}, \\
& \sum_{i=1}^{m} \alpha_i^* y^{(i)} = 0, \\
& \alpha_i^* \left( 1 - y^{(i)} \left( w^*^T s^{(i)} + b^*^T x^{(i)} + c^* \right) \right) = 0, \quad i = 1, \ldots, m, \\
& \alpha^* \geq 0 \\
& 1 - y^{(i)} \left( w^*^T s^{(i)} + b^*^T x^{(i)} + c^* \right) \leq 0, \quad i = 1, \ldots, m.
\end{align*}
\] (12)

Note that (5) implies that (L1-QSSVM') has strictly feasible solutions, i.e., there exists $(\bar{w}, \bar{b}, \bar{c})$ such that

\[
1 - y^{(i)} \left( \bar{w}^T s^{(i)} + \bar{b}^T x^{(i)} + \bar{c} \right) > 1, \quad i = 1, \ldots, m.
\]

Therefore, by Exercise 5.3.1 in [1], we know that the set of Lagrangian multipliers $\alpha^*$ is bounded from above. In particular, we have

\[
\|\alpha^*\|_1 \leq \pi \triangleq \frac{q(\bar{w}, \bar{b}, \bar{c}) - q^*}{c_1},
\] (13)

where $q^*$ is the optimal value of (L1-QSSVM') and $c_1 = \min_{i=1, \ldots, m} \left[ y^{(i)} \left( \bar{w}^T s^{(i)} + \bar{b}^T x^{(i)} + \bar{c} \right) - 1 \right]$.

**Theorem 4.5.** Assume the data set $\mathcal{D}$ is quadratically separable and the matrix $G$ is positive definite. For any $\lambda$, there exists a $\mu$ (depending on $\lambda$), such that for all $\mu > \mu$, (L1-SQSSVM') has a unique solution $(w^*, b^*, c^*, \xi^*)$ with $\xi^* = 0_m$.

**Proof.** We start with taking an optimal solution of (L1-QSSVM'), say $(w^*, b^*, c^*)$ and then construct an optimal solution of (L1-SQSSVM'). It is clear that the KKT conditions for convex problem (L1-SQSSVM') yields the necessary and sufficient conditions for optimality. Let $\alpha^*$ be a vector of multipliers such that $(w^*, b^*, c^*, \alpha^*)$ satisfies (12). Let

$$
\mu > \pi,
$$
where $\pi$ is defined in (13). Notice that $\pi$ depends on $\lambda$. It is clear that $\mu > \|\alpha^*\|_\infty$. For any $\mu > \mu^*$, we let $\eta^* = \mu 1_m - \alpha^*$. By the definition of $\mu$, it is clear that $\eta^* \geq 0$. It suffices to verify that $(w^*, b^*, c^*, \xi^* = 0_m, \alpha^*, \eta^*)$ satisfies the following KKT conditions:

$$
\begin{align*}
0 &\in 2 \sum_{i=1}^m M^{(1)}_i M^{(1)} w^* + 2 \sum_{i=1}^m M^{(1)}_i b^* + \lambda \partial (\|\cdot\|_1) w^* - \sum_{i=1}^m \alpha^*_i y^{(i)} s^{(i)}, \\
2 \sum_{i=1}^m M^{(1)} w^* + 2mb^* &= \sum_{i=1}^m \alpha^*_i y^{(i)} x^{(i)}, \\
\sum_{i=1}^m \alpha^*_i y^{(i)} &= 0, \\
\alpha^*_i \left(1 - \xi^*_i - y^{(i)} \left(w^* T s^{(i)} + b^* T x^{(i)} + c^*\right)\right) &= 0, \quad i = 1, \ldots, m, \\
\alpha^* &\geq 0, \\
1 - \xi^*_i - y^{(i)} \left(w^* T s^{(i)} + b^* T x^{(i)} + c^*\right) &\leq 0, \quad i = 1, \ldots, m, \\
\xi^*_i \eta^*_i &= 0 \quad i = 1, \ldots, m, \\
\xi^* &\geq 0, \\
\eta^* &> 0, \\
\mu &= \alpha^* + \eta^*, \quad i = 1, \ldots, m.
\end{align*}
$$

Since $(w^*, b^*, c^*, \alpha^*)$ satisfies (12), it is straightforward to verify that $(w^*, b^*, c^*, \xi^* = 0_m, \alpha^*, \eta^*)$ satisfies (14) and hence is an optimal solution of L1-SQSSVM. Since $G$ is positive definite, we know that $w^*$ and $b^*$ is unique by Theorem 4.2. And since $(c^*, \xi^*)$ must be an optimal solution of linear program (11), we conclude that $\xi^* = 0_m$ is the only solution. By a similar argument for Theorem 5 in [12], $c^*$ is also unique. This concludes the proof.

**Remark.** Theorem 4.5 can be extended to the original SQSSVM models studied in [12], leading to a result stronger than Theorem 2 therein for which the parameter $\mu$ must go to infinity.

### 4.3 Effects of $\ell_1$ Norm Regularization

We next study the effects of $\ell_1$ norm regularization. First, we consider the case when the training data set $\mathcal{D}$ defined in (4) is linearly separable according to (6). As we have discussed, in this case, it is desirable that the QSSVM returns a separation hyperplane rather than a quadratic surface. But there is no guarantee to have such property for this model. On the other hand, our proposed model (L1-QSSVM) captures this desired property for a finite but large enough $\lambda$. Mathematically, this is equivalent to $w^* = 0$ in an optimal solution of (L1-QSSVM) for some $\lambda$. To show this, we start with an optimal solution of the standard SVM. Consider the following standard SVM with hard margin:

$$
\begin{align*}
\min_{u,d} \quad &\frac{1}{2} \|u\|_2^2 \\
\text{s.t.} \quad &y^{(i)} (u^T x^{(i)} + d) \geq 1, \quad i = 1, \ldots, m, \\
&u \in \mathbb{R}^n, d \in \mathbb{R}.
\end{align*}
$$

(SVM)

Under the linear separability assumption (6), the standard SVM with hard margin (SVM) is feasible, and the objective function is bounded from below. Therefore, there exists an optimal solution $(u^*, d^*)$ that solves (SVM). The Lagrangian of (SVM) is the following:

$$
\mathcal{L}_{\text{SVM}} (u, d, \beta) = \frac{1}{2} \|u\|_2^2 + \sum_{i=1}^m \beta_i \left(1 - y^{(i)} (u^T x^{(i)} + d)\right),
$$

(15)
where $\beta = [\beta_1, \beta_2, \ldots, \beta_m]^T$ are the Lagrangian multipliers. It is clear that the necessary and sufficient condition for $(u^*, d^*)$ to be an optimal solution of (SVM) is the existence of a Lagrangian multipliers vector $\beta^*$ such that the following KKT conditions are satisfied:

\[
\begin{aligned}
& u^* = \sum_{i=1}^{m} \beta_i^* y^{(i)} x^{(i)}, \\
& \sum_{i=1}^{m} \beta_i^* y^{(i)} = 0, \\
& \beta_i^* \left(1 - y^{(i)} (u^T x^{(i)} + d^*)\right) = 0, \quad i = 1, \ldots, m, \\
& \beta_i^* \geq 0, \quad i = 1, \ldots, m, \\
& 1 - y^{(i)} (u^T x^{(i)} + d) \leq 0, \quad i = 1, \ldots, m.
\end{aligned}
\] (16)

In the next theorem, we show that $(0_{n \times m}, u^*, d^*)$ in fact solves (L1-QSSVM) when $\lambda$ is large enough.

**Theorem 4.6 (Equivalence of SVM and L1-QSSVM for finite $\lambda$).** Suppose that the training data set $\mathcal{D}$ defined in (4) is linearly separable (as defined in (6)). Let $(u^*, d^*, \beta^*)$ satisfy the KKT conditions (16), then $W^* = 0_{n \times m}$, $b^* = u^*$, $c^* = d^*$, solves (L1-QSSVM) when $\lambda$ is large enough.

**Proof.** For convenience, we consider the equivalent formulation (L1-QSSVM$''$). The Lagrangian of (L1-QSSVM$''$) is the following:

\[
\mathcal{L}_Q(w, b, c, \alpha) = \sum_{i=1}^{m} w^T M^{(i)} T M^{(i)} w + 2 \sum_{i=1}^{m} w^T M^{(i)} b + mb^T b + \lambda \|w\|_1 + \sum_{i=1}^{m} \alpha_i \left(1 - y^{(i)} (w^T s^{(i)} + b^T x^{(i)} + c)\right).
\] (17)

The optimality KKT conditions for this problem based on (3) are as follows:

\[
\begin{aligned}
& 0 \in 2 \sum_{i=1}^{m} M^{(i)} T M^{(i)} w^* + 2 \sum_{i=1}^{m} M^{(i)} T b^* + \lambda \partial (\|\cdot\|_1)|_{w^*} - \sum_{i=1}^{m} \alpha_i^* y^{(i)} s^{(i)}, \\
& 2 \sum_{i=1}^{m} M^{(i)} w^* + 2mb^* = \sum_{i=1}^{m} \alpha_i^* y^{(i)} x^{(i)}, \\
& \sum_{i=1}^{m} \alpha_i^* y^{(i)} = 0, \\
& \alpha_i^* \left(1 - y^{(i)} (w^* s^{(i)} + b^* x^{(i)} + c^*)\right) = 0, \quad i = 1, \ldots, m, \\
& \alpha_i^* \geq 0, \quad i = 1, \ldots, m, \\
& 1 - y^{(i)} (w^* s^{(i)} + b^* x^{(i)} + c^*) \leq 0, \quad i = 1, \ldots, m.
\end{aligned}
\] (18)

From (16), one can see that \[ [u^* T \quad b^* T \quad c^* \quad \alpha^* T] = [0^T \quad u^* T \quad d^* \quad 2m\beta^T] \] satisfies all the equations in (18) except $0 \in \frac{\partial \mathcal{L}_Q}{\partial w} \bigg|_0$. Nevertheless, this condition is equivalent to

\[
\left\| \sum_{i=1}^{m} M^{(i)} T u^* - \sum_{i=1}^{m} \beta_i^* y^{(i)} s^{(i)} \right\|_\infty \leq \frac{\lambda}{2}.
\] (19)

So, if we choose $\lambda$ large enough, this condition also holds. Hence, \[ [0^T \quad u^* T \quad d^* \quad 2m\beta^T] \] satisfies the KKT conditions when $\lambda$ is large enough. Since the KKT conditions are also sufficient for convex program, we conclude that $W^* = 0_{n \times m}$, $b^* = u^*$, $c^* = d^*$, solves (L1-QSSVM). \qed
Next, we find a lower bound for such $\lambda$. From the inequality (19), it is enough to find an upper bound for
\[
\left\| \sum_{i=1}^{m} \mathbf{M}^{(i)T} \mathbf{u}^{*} - m \sum_{i=1}^{m} \beta_{i}^{*} y^{(i)} s^{(i)} \right\|_{\infty},
\]
where $\mathbf{u}^{*}$ and $\beta^{*}$ satisfy (16). Let
\[
a = \sum_{i=1}^{m} \mathbf{M}^{(i)T} \mathbf{u}^{*} - m \sum_{i=1}^{m} \beta_{i}^{*} y^{(i)} s^{(i)} \in \mathbb{R}^{n(n+1)/2}.
\]
By denoting $\mathbf{T} := \mathbf{X}^T \text{Diag}(\mathbf{y})$, we have $\mathbf{u}^{*} = \sum_{i=1}^{m} \beta_{i}^{*} y^{(i)} \mathbf{x}^{(i)} = \mathbf{T} \beta^{*}$ so that
\[
\| \mathbf{u}^{*} \|_{2} \leq \| \mathbf{T} \|_{2} \| \beta^{*} \|_{2} = \| \mathbf{X}^T \|_{2} \| \beta^{*} \|_{2} = \| \mathbf{X} \|_{2} \| \beta^{*} \|_{2} \leq \| \mathbf{X} \|_{2} \| \beta^{*} \|_{1}.
\]
Thus, along with definitions of (3.1) and (3.4), for $k \in \{1, 2, \ldots, n(n+1)/2\}$, we have:
\[
|a_k| \leq \sum_{i=1}^{m} \| \mathbf{M}_{k}^{(i)} \|_{2} \| u^{*} \|_{2} + m \sum_{i=1}^{m} \| \beta_{i}^{*} \|_{\infty} | s_{k}^{(i)} |
\]
\[
\leq \sum_{i=1}^{m} \| \mathbf{x}^{(i)} \|_{2} \| u^{*} \|_{2} + m \sum_{i=1}^{m} \| \beta_{i}^{*} \|_{\infty} \| \mathbf{x}^{(i)} \|_{\infty}^{2}
\]
\[
\leq m \| u^{*} \|_{2} \max_{i} \| \mathbf{x}^{(i)} \|_{2} + m \| \beta^{*} \|_{1} \max_{i} \| \mathbf{x}^{(i)} \|_{\infty}^{2}
\]
\[
\leq m \| \mathbf{X} \|_{2} \| \beta^{*} \|_{1} \max_{i} \| \mathbf{x}^{(i)} \|_{2} + m \| \beta^{*} \|_{1} \max_{i} \| \mathbf{x}^{(i)} \|_{\infty}^{2}
\]
\[
= m \| \beta^{*} \|_{1} \left( \| \mathbf{X} \|_{2} \max_{i} \| \mathbf{x}^{(i)} \|_{2} + \max_{i} \| \mathbf{x}^{(i)} \|_{\infty}^{2} \right).
\]
It suffices to find an upper bound for $\| \beta^{*} \|_{1}$. Note that (6) implies that (SVM) has strictly feasible solutions, i.e., there exists $(\mathbf{u}, \mathbf{d})$ such that
\[
y^{(i)} (\mathbf{u}^T \mathbf{x}^{(i)} + \mathbf{d}) > 1, \quad i = 1, \ldots, m.
\]
Therefore, by Exercise 5.3.1 in [1], we know that the set of Lagrangian multipliers $\beta^{*}$ is bounded from above. In particular, we have
\[
\| \beta^{*} \|_{1} \leq \frac{\| \mathbf{u} \|_{2}^{2} - \| \mathbf{u}^{*} \|_{2}^{2}}{2c_{2}} \leq \frac{\| \mathbf{u} \|_{2}^{2}}{2c_{2}},
\]
where $c_{2} = \min_{i=1, \ldots, m} \left[ y^{(i)} (\mathbf{u}^T \mathbf{x}^{(i)} + \mathbf{d}) - 1 \right]$. Thus, to have the above result, it suffices to have
\[
\lambda \geq m \frac{\| \mathbf{u} \|_{2}^{2}}{2c_{2}} \left( \| \mathbf{X} \|_{2} \max_{i} \| \mathbf{x}^{(i)} \|_{2} + \max_{i} \| \mathbf{x}^{(i)} \|_{\infty}^{2} \right).
\]

We can show a similar result for the soft margin version. We consider the soft margin version of SVM as follows.
\[
\min_{\mathbf{u}, \mathbf{d}, \boldsymbol{\xi}} \frac{1}{2} \| \mathbf{u} \|_{2}^{2} + \mu \sum_{i=1}^{m} \xi_{i}
\]
\[
s.t. \quad y^{(i)} (\mathbf{u}^T \mathbf{x}^{(i)} + \mathbf{d}) \geq 1 - \xi_{i}, \quad i = 1, \ldots, m,
\]
\[
\mathbf{u} \in \mathbb{R}^{n}, \mathbf{d} \in \mathbb{R}, \boldsymbol{\xi} \in \mathbb{R}^{m}_{+}.
\]
Since (SSVM) is always feasible and the objective value is bounded from below, there exists an optimal solution $(\mathbf{u}^{*}, d^{*}, \boldsymbol{\xi}^{*})$. We can show the following result.
**Corollary 4.6.1.** Let \((u^*, d^*, \xi^*)\) be an optimal solution of (SSVM). It follows that 
\[
(0_{n \times n}, u^*, d^*, \xi^*)
\]
solves (L1-SQSSVM) when \(\lambda\) is large enough.

Next we consider the case when the data is quadratically separable with a sparse matrix \(W\). In particular, we assume that the data set is separable by quadratic function \(f(x) = \frac{1}{2}x^T W x + b^T x + c\), where \(w = \text{hvec}(W)\) contains mostly 0’s. Let \(\mathcal{Z}\) be the set of indices of 0’s in \(w\), i.e., \(w_j = 0\) for all \(j \in \mathcal{Z}\). In this case, the following restricted (QSSVM) model is feasible and has an optimal solution with a finite objective value:

\[
\begin{align*}
\min_{w, b, c} & \quad q(w, b, c) \triangleq \sum_{i=1}^{m} w^T M^{(i)}^T M^{(i)} w + 2 \sum_{i=1}^{m} w^T M^{(i)} b + m b^T b \\
\text{s.t.} & \quad y^{(i)} \left( w^T s^{(i)} + b^T x^{(i)} + c \right) \geq 1, \quad i = 1, \ldots, m, \\
& \quad w_j = 0, \quad \forall j \in \mathcal{Z}, \\
& \quad w \in \mathbb{R}^{n(n+1)/2}, \quad b \in \mathbb{R}^n, \quad c \in \mathbb{R}.
\end{align*}
\]

Let \((w^*, b^*, c^*)\) be an optimal solution of (R-QSSVM’), there exist multipliers \(\alpha^* \in \mathbb{R}^m\), and \(\beta^*_\mathcal{Z} \in \mathbb{R}^{n(n+1)/2}\), such that the KKT conditions are satisfied. We expand \(\beta^*_\mathcal{Z}\) to \(\beta^* \in \mathbb{R}^{n(n+1)/2}\) by filling 0’s at the indices not in \(\mathcal{Z}\), the KKT conditions can be written below:

\[
\begin{align*}
2 \sum_{i=1}^{m} M^{(i)}^T M^{(i)} w^* + 2 \sum_{i=1}^{m} M^{(i)} b^* - \sum_{i=1}^{m} \alpha^*_i y^{(i)} s^{(i)} + \beta^* &= 0, \\
2 \sum_{i=1}^{m} M^{(i)} w^* + 2 m b^* &= \sum_{i=1}^{m} \alpha^*_i y^{(i)} x^{(i)}, \\
\sum_{i=1}^{m} \alpha^*_i y^{(i)} &= 0, \\
\alpha^*_i \left( 1 - y^{(i)} \left( w^*^T s^{(i)} + b^*^T x^{(i)} + c^* \right) \right) &= 0, \quad i = 1, \ldots, m, \\
\alpha^* &\geq 0, \\
1 - y^{(i)} \left( w^*^T s^{(i)} + b^*^T x^{(i)} + c^* \right) &\leq 0, \quad i = 1, \ldots, m, \\
w_j &= 0, \quad \forall j \in \mathcal{Z}.
\end{align*}
\]

Similar to Theorem 4.6, we can see that when \(\lambda > \|\beta^*\|_{\infty}\), \((w^*, b^*, c^*, \alpha^*)\) satisfies the KKT conditions (18), and hence \((w^*, b^*, c^*)\) is an optimal solution of (L1-QSSVM). This indicates, that when \(\lambda\) is large enough, the \(\ell_1\) norm regularization can accurately capture the sparsity in matrix \(W\).

The above argument can also be applied for the model L1-SQSSVM over any given data set. However, we can have a stronger result in quadratically separable case. In fact, by combining this result with the ones obtained from Theorems 4.2, 4.4, 4.5, when the separating quadratic surface is generated by a sparse matrix \(W\), we have the below corollary.

**Corollary 4.6.2.** For almost any quadratically separable (5) data set \(\mathcal{D}\) (4) for which the generating matrix \(W^*\) is sparse, the proposed model L1-SQSSVM obtains a unique solution that captures this sparse matrix \(W^*\) and also \(\xi^* = 0\) provided that penalty parameters \(\lambda\) and \(\mu\) are large enough.

### 5 Numerical Experiments on Performance of L1-QSSVM and L1-SQSSVM

In this section, we conduct various numerical experiments to analyze the behavior of L1-QSSVM and L1-SQSSVM over different data sets and demonstrate their effectiveness. All the experiments are
conducted on a server with 64 Intel(R) Xeon(R) CPU E5-2686 v4 @ 2.30GHz CPUs and 480G RAM. We use Gurobi 7.0.2 to solve the quadratic programs in all the QSSVM models.

Figure (1b) depicts the flexibility of L1-QSSVM in capturing linear and quadratic separating surfaces. When data set is linearly separable (1b), L1-QSSVM yields a hyperplane for $\lambda = 10000$ but when it is quadratically separable (1b), L1-QSSVM with $\lambda = 1$ behaves exactly the same as QSSVM. Nonetheless, this figure confirms that SVM does not perform well when the data set is quadratically separable unlike their success in linearly separable data sets.

Figure 1: L1-QSSVM performance on linearly and quadratically separable data sets.

Figure 2 verifies Corollary 4.6.1 on L1-SQSSVM in visual details. Given a linearly separable data set and fix $\mu$, we plot the separating surfaces obtained from L1-SQSSVM for different values of $\lambda$ along with the separating surfaces obtained from SVM and SQSSVM. We can see that when $\lambda$ is small, the solution of L1-SQSSVM is close to that of SQSSVM and when $\lambda$ is large, the solution of L1-SQSSVM is close to that of SVM. In other words, as $\lambda$ gets bigger, the solution of L1-SQSSVM becomes flatter. Roughly speaking, the curvature approaches zero.

We bring Figure 3a to numerically verify Theorem 4.5. As shown in both pictures, optimal solution of L1-SQSSVM approaches to that of L1-QSSVM as $\mu$ becomes large enough.

Figure 2: Influence of parameter $\lambda$ on curvature of optimal solution of L1-SQSSVM.
Next, we numerically demonstrate that the $\ell_1$ norm term in our proposed models is significant in classification, namely, a suitable parameter $\lambda > 0$ exists that leads to a better performance than $\lambda = 0$. We only focus on the soft margin model because both models resemble similar behaviour in this sense. To show the existence of this optimum parameter $\lambda$ is independent of the choice of parameter $\mu$ and data set, we have six different data sets in which fixed parameter $\mu$ changes from small to large. To tune a suitable approximation of optimum parameter $\lambda$, we use SQSSVM for a given data set and then $\hat{\mu}$ with a highest accuracy score is adopted. Note that our model has two parameters (one more degree of freedom than that of SQSSVM) so that it naturally improves the accuracy of classification compared with SQSSVM with $\hat{\mu}$. The considered discrete range for $\mu$ to obtain $\hat{\mu}$ is such that $\log_2 \mu \in \{-3, -2, \ldots, 20\}$. If distinct values of $\hat{\mu}$ exist, we simply set up $\hat{\mu}$ as their mean. Figure 4 depicts that for different scales of $\hat{\mu}$, our proposed model L1-SQSSVM for some $\lambda > 0$ reaches a better performance than of its parental model SQSSVM in which $\lambda = 0$ on artificial and real world data sets.

Consider the case where a given data set is quadratically separable with a sparse $W$ matrix, i.e., when the separation surface $f(x) = \frac{1}{2}x^T W x + b^T x + c = 0$ has a sparse $W$. By applying L1-SQSSVM
one can see that the $\ell_1$ norm regularization term enforces detecting the true sparsity pattern of this matrix. To demonstrate this property experimentally, we first generate a quadratic surface using 10 features with the following sparse matrix $W$, and vector $b$ and constant $c$:

$$
W = \begin{bmatrix}
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 \\
0 & 2 & 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 \\
0 & 0 & 3 & 0 & 0 & 0 & 5 & 0 & 0 & 0 \\
0 & 0 & 0 & 4 & 0 & 0 & 0 & 6 & 0 & 0 \\
0 & 0 & 0 & 5 & 0 & 0 & 0 & 7 & 0 & 0 \\
0 & 0 & 0 & 0 & 6 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 7 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix},
$$

$$
b = \begin{bmatrix}
1 \\
\vdots \\
1 \\
-1
\end{bmatrix},
$$

$c = 2.$ (20)

We next randomly generate 200 data points on each side of the resulting quadratic separating surface and another 100 noisy data points around this surface. Then, using the same idea as explained before, we utilize SQSSVM on this data set to tune parameter $\mu$ and obtain the best $\hat{\mu}$; in terms of accuracy score. We finally apply L1-SQSSVM with this $\hat{\mu}$ and obtain their optimal matrices as $\lambda$ varies. Figure 5 shows that the sparsity of $W$ in (20) is captured as parameter $\lambda$ becomes larger.

![Figure 5: Sparsity pattern detection using L1-SQSSVM as parameter $\lambda$ varies.](image)

Lastly, in order to test the classification accuracy and efficiency of L1-SQSSVM, we use two benchmark data sets from UCI repository for our experiments. Since our focus is on binary classification, if one of these data sets contains more than two classes, we only choose two of them. A description of the data sets used can be found in Table 1. We compare our L1-SQSSVM with SQSSVM, SVM, and SVM with a Quadratic kernel (SVM-Quad) models. For SVM-Quad we used SVC with 2-degree polynomial kernel Python package *Scikit-learn* [18]. We randomly pick $k\%$ of the full data set for its training and apply the grid method to find the best parameters of $\mu$ for L1-SQSSVM, SQSSVM, SVM and SVM-Quad), and $\lambda$ for (L1-SQSSVM). The parameter used inside the quadratic kernel is selected by the package over training the full data set. As reported in [5, 12], training rate $k$ is set to be 10, 20 and 40. In order to be statistically meaningful, for each fixed training rate $k$ on each model, the experiments are repeated for 50 times. The mean, standard deviation, the minimum and the maximum of accuracy scores, and the average CPU time among these 50 experiments are recorded. The accuracy score is defined as the rate of achieved correct labels by the model over the full data set. Note that the CPU time recorded in this paper does not include the time for tuning parameters.
| Data set     | # of features | name of class   | sample size |
|--------------|---------------|-----------------|-------------|
| Iris         | 4             | Versicolour     | 50          |
|              |               | Virginica       | 50          |
| Car evaluation | 6            | unacc           | 1210        |
|              |               | acc             | 384         |

Table 1: Description of 2-class data sets used.

| Training Rate k% | Model       | Accuracy score (%) | CPU time (s) |
|------------------|-------------|--------------------|--------------|
|                  |             | mean    | std     | min    | max    |          |
| 10               | L1-SQSSVM   | 91.93   | 5.49    | 63.33  | 98.89  | 0.067    |
|                  | SQSSVM      | 89.33   | 4.07    | 81.11  | 96.67  | 0.067    |
|                  | SVM-Quad    | 89.49   | 4.91    | 80.00  | 97.78  | 0.001    |
|                  | SVM         | 89.62   | 4.10    | 78.89  | 97.78  | 0.001    |

Table 2: Iris results.

| Training Rate k% | Model       | Accuracy score (%) | CPU time (s) |
|------------------|-------------|--------------------|--------------|
|                  |             | mean    | std     | min    | max    |          |
| 20               | L1-SQSSVM   | 94.33   | 2.20    | 90.00  | 98.75  | 0.079    |
|                  | SQSSVM      | 92.60   | 2.57    | 82.50  | 96.25  | 0.078    |
|                  | SVM-Quad    | 93.03   | 2.72    | 86.25  | 98.75  | 0.001    |
|                  | SVM         | 93.00   | 3.01    | 82.50  | 97.50  | 0.001    |

Table 3: Car evaluation results.

From Tables 2 and 3, we observe that not only the mean accuracy scores obtained by L1-SQSSVM are the same or better than those of other models over either the iris data or car evaluation data sets, but also the elapsed CPU times reported are reasonable.
6 Conclusion

This paper generalizes the standard kernel-free models of linear and quadratic surface support vector machines. The SVMs are only designed for (almost) linearly separable data sets and the QSSVMs just work for (almost) quadratically separable data sets; without reducing to the corresponding hard or soft margin SVM if the data set is linearly separable. In other words, when the actual $W = 0$, the QSSVMs often output a surface with $W^* \neq 0$, which is a discouragement for such generalizations of SVMs.

By incorporating an $\ell_1$ norm regularization in the objective function, we propose L1-QSSVM models that not only resolve these shortcomings but also capture possible sparsity pattern for appropriate penalty parameters. We further establish other interesting theoretical results such as solution existence, uniqueness, and vanishing margin for the soft margin version if the penalty parameter is large enough. To conclude the paper, we summarize all the obtained theoretical results for different types of data sets in the table below.

| Data set                | Model          | L1-QSSVM                                      | L1-SQSSVM                                    |
|-------------------------|----------------|-----------------------------------------------|----------------------------------------------|
| Linearly Separable      | L1-QSSVM       | • Solution existence                          | • Solution existence                          |
|                         |                | • $z^*$ is almost always unique                | • $z^*$ is almost always unique               |
|                         |                | • Equivalence with SVM for large enough $\lambda$ | • Equivalence with SSVM for large enough $\lambda$ |
|                         |                |                                               | • Solution is almost always unique with $\xi^* = 0$ for large enough $\mu$ |
| Quadratically Separable | L1-QSSVM       | • Solution existence                          | • Solution existence                          |
|                         |                | • $z^*$ is almost always unique                | • $z^*$ is almost always unique               |
|                         |                | • Capturing possible sparsity of $W^*$ for large enough $\lambda$ | • Solution is almost always unique with $\xi^* = 0$ for large enough $\mu$ |
|                         |                |                                               | • Capturing possible sparsity of $W^*$ for large enough $\lambda$ |
| Neither                 |                |                                               | • Solution existence                          |
|                         |                |                                               | • $z^*$ is almost always unique               |

Figure 6: Summary of obtained theoretical results in the paper.

Therefore, along with the promising practical efficiency of these models demonstrated in Section 5, we conclude that the proposed L1-QSSVMs are justifiable in theory and effective in practice.

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