A Semismooth-Newton’s-Method-Based Linearization and Approximation Approach for Kernel Support Vector Machines

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Received: date / Accepted: date

Abstract Support Vector Machines (SVMs) are among the most popular and the best performing classification algorithms. Various approaches have been proposed to reduce the high computation and memory cost when training and predicting based on large-scale datasets with kernel SVMs. A popular one is the linearization framework, which successfully builds a bridge between the $L_1$-loss kernel SVM and the $L_1$-loss linear SVM. For linear SVMs, very recently, a semismooth Newton’s method is proposed. It is shown to be very competitive and have low computational cost. Consequently, a natural question is whether it is possible to develop a fast semismooth Newton’s algorithm for kernel SVMs. Motivated by this question and the idea in linearization framework, in this paper, we focus on the $L_2$-loss kernel SVM and propose a semismooth Newton’s method based linearization and approximation approach for it. The main idea of this approach is to first set up an equivalent linear SVM, then apply the Nyström method to approximate the kernel matrix, based on which a reduced linear SVM is obtained. Finally, the fast semismooth Newton’s method is employed to solve the reduced linear SVM. We also provide some theoretical analyses on the approximation of the kernel matrix. The advantage of the proposed approach is that it maintains low computational cost and keeps a fast convergence rate. Results of extensive numerical experiments verify the efficiency of the proposed approach in terms of both predicting accuracy and speed.

Keywords Support vector machines · Kernel methods · Semismooth Newton’s methods · Nyström methods

1 Introduction

Support Vector Machines (SVMs) [Cortes and Vapnik 1995, Xie and Xu 2019] are among the most popular and the best performing classification algorithms. SVMs have been successfully used in vari-

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This author’s research was supported by the National Natural Science Foundation of China (No.11671036).
uous applications such as test classification (Tong and Kolter 2001; Zhang et al. 2008), computational biology (Schölkopf et al. 2004; Huang et al. 2018) and finance (Chen and Hao 2017). For data with linear boundaries, the linear SVMs aim to generate an optimal separating hyperplane between the two classes. Kernel methods (Schölkopf et al. 2002) map the input data into the reproducing kernel Hilbert space (RKHS), which allow Kernel SVMs to abstract the nonlinear relations in the input data. While kernel SVMs provide powerful tools to solve classification problems with various input data, there are also challenges in designing algorithms for kernel SVMs. The first challenge is how to compute and save the kernel matrix, which is usually dense (Shin and Cho 2005; Feng and Liao 2017). In addition to that, in kernel SVMs, the number of support vectors that have to be explicitly maintained grows linearly with the sample size on noisy data, which is referred to as the curse of kernelization (Wang et al. 2010).

Various approaches have been proposed to reduce the high computation and memory cost when training and predicting based on large-scale datasets with kernel SVMs such as SVMperf (Joachims and Yu 2009), Pegasos (Shalev-Shwartz et al. 2011), budgeted stochastic gradient descent (BSGD) (Wang et al. 2012; Djuric et al. 2013) and the widely used LIBSVM (Chang and Lin 2011). However, due to the data explosion in the past few years, efficient algorithms for large-scale kernel SVMs are still highly in need.

**Related Works.** One popular way to deal with large-scale kernel SVMs is the linearization framework (Zhang et al. 2012), which successfully builds a bridge between the $L_1$-loss kernel SVM and the $L_1$-loss linear SVM. The linearization framework enables us to linearize the kernel SVM through approximation and decomposition of the kernel matrix and solving it with linear solvers, so that solving large-scale kernel SVMs can also benefit from the advanced and extremely efficient linear SVMs’ solvers. Inspired by the idea of Zhang et al. (2012), efforts have been made to improve the approximation of the kernel matrix under the linearization framework, such as memory efficient kernel approximation (Si et al. 2017) and Hash-SVM (Mu et al. 2014).

One of the attractive properties of the linearization framework is that it provides us a way to solve kernel SVMs by various linear SVMs’ solvers. A variety of methods have been proposed, including the popular trust region Newton method (TRON) (Lin et al. 2008) and the dual coordinate descent method (DCD) (Hsieh et al. 2008). Recently, there has been great progress on algorithms for linear SVMs with large-scale datasets (Yuan et al. 2012), for instance the stochastic gradient descent method (Zhang 2004), the cutting plane method (Joachims 2004), SVM-ALM algorithm (Nie et al. 2014), the fast APG (FAPG) method (Ito et al. 2017) as well as the recent AL-SNCG method (Yan and Li 2019). We refer to Chauhan et al. (2019) for monographs and reviews on linear SVMs. In particular, a semismooth Newton’s method (Yin and Li 2019) is proposed very recently, which is shown to be very competitive and have low computational cost. Consequently, a natural question is whether it is possible to develop a fast semismooth Newton’s algorithm for kernel SVMs.

**Our Contributions.** Motivated by this question and the idea in linearization framework, in this paper, we focus on the $L_2$-loss kernel SVM and propose a semismooth Newton’s method based linearization and approximation approach for it. The main idea of this approach is to first set up an equivalent linear SVM, then apply the Nyström method to approximate the kernel matrix, based on which a reduced linear SVM is obtained. We also provide some theoretical analyses on the approximation of the kernel matrix. Finally, the fast semismooth Newton’s method is employed to solve the reduced linear SVM. The advantage of the proposed approach is that it maintains low computational cost and keeps a fast convergence rate. Results of extensive numerical experiments verify the efficiency of the proposed approach in terms of both predicting accuracy and speed.

The rest of the paper is organized as follows. In Section 2, we present the kernel SVMs and a brief review about linearized kernel SVM proposed by Zhang et al. (2012). In Section 3 we introduce the linearization and approximation approach. In Section 4 we analyze the theoretical error of approxi-
imation for the kernel matrix. In Section 5 we apply the fast semismooth Newton’s method for the reduced linear SVMs. In Section 6 we conduct numerical tests to verify the efficiency of our approach. Final conclusions are given in Section 7.

Notations We use bold letters to indicate vectors and matrices, and \( \| \cdot \| \) to denote the \( l_2 \) norm for vectors and Frobenius norm for matrices. Let \( \mathbb{S}^n \) denote the space of \( n \times n \) symmetric matrices.

2 Preliminaries

2.1 Kernel SVMs

The SVMs can be divided into support vector machine classifiers and support vector regression (SVR) models due to different purposes. In our paper, we focus on SVM classifiers and our method is also applicable to SVR models.

Given training data consists of \( n \) pairs \( (x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n) \), with \( x_i \in \mathbb{R}^p \) and \( y_i \in \{ -1, 1 \} \), the idea of kernel SVMs is to map the training data from the input space \( \mathbb{R}^p \) to a Hilbert space \( \mathcal{Y} \) by a feature mapping function \( \psi : \mathbb{R}^p \to \mathcal{Y} \), where \( \mathcal{Y} \) is the feature space. The kernel SVMs are to train the following model

\[
\min_{w, b} \frac{1}{2} \|w\|^2 + C \hat{R}(w, b),
\]

where \( C \) is some positive constant, \( \hat{R}(w, b) = \frac{1}{n} \sum_{i=1}^{n} L(w, b; \psi(x_i), y_i) \) is the empirical error, with \( L(\cdot) \) being the loss function. Denote that \( C = C_0/n \) is the cost parameter. A special case is that when \( \psi \) is an identity mapping, i.e., \( \psi(x) = x \), then kernel SVMs reduce to the linear SVMs.

Denote

\[
X_e = \begin{bmatrix} x_1^T \\ \vdots \\ x_n^T \end{bmatrix} \in \mathbb{R}^{n \times p}, \quad y_e = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} \in \mathbb{R}^n, \quad X_e = \begin{bmatrix} x_{n+1}^T \\ \vdots \\ x_{n+m}^T \end{bmatrix} \in \mathbb{R}^{m \times p},
\]

where \( X_e \) is the test dataset. Three popular choices for \( L(\cdot) \) are the \( L_1 \)-loss function, \( L_2 \)-loss function and logistic function. In our paper, we focus on the \( L_2 \)-loss kernel SVM, i.e.,

\[
\min_{w, b} \frac{1}{2} \|w\|^2 + C \sum_{i=1}^{n} \max(0, y_i(\psi(x_i)^T w + b))^2.
\]

It can be equivalently written as

\[
\min_{w, b} \frac{1}{2} \|w\|^2 + C \sum_{i=1}^{n} \xi_i^2 \\
\text{s.t.} \quad y_i(w^T \psi(x_i) + b) \geq 1 - \xi_i, \quad \xi_i \geq 0, \quad i = 1, \ldots, n.
\]

with the dual problem

\[
\max_{\lambda \in \mathbb{R}^n} \lambda^T e - \frac{1}{2} \lambda^T Q \lambda - \frac{1}{2c} \|\lambda\|^2 \\
\text{s.t.} \quad \lambda^T y = 0, \quad \lambda \geq 0,
\]

where \( Q \in \mathbb{S}^n \) is defined by \( Q_{ij} = y_i y_j \langle \psi(x_i), \psi(x_j) \rangle \), \( i, j = 1, \ldots, n \).

Let \((w^*, b^*)\) be the optimal solution of (1). The predicting label for testing data \( x \in \mathbb{R}^p \) is

\[
\text{sign}((w^*)^T \psi(x) + b^*).
\]
Let $\mathbf{w}^*$ be the optimal solution of (5), there is $\mathbf{w}^* = \sum_i \lambda_i \psi(x_i)$, and the predicting label becomes

$$\text{sign}(\sum_i y_i \lambda_i \langle \psi(x_i), \psi(x) \rangle + b^*).$$

(7)

Given the fact that $\psi$ may be an infinite mapping, it may not be easy to give $\psi$ explicitly. Since (5) and (7) involve $\psi(x)$ only through the inner product, one can define the kernel function $\kappa : \mathbb{R}^p \times \mathbb{R}^p \rightarrow \mathbb{R}$ instead, by $\kappa(x, x') = \langle \psi(x), \psi(x') \rangle$. Popular kernel functions (Hastie et al. 2005) include

- $d$th-degree polynomial: $\kappa(x, x') = (1 + \langle x, x' \rangle)^d$,
- radial basis: $\kappa(x, x') = \exp(-\gamma \|x - x'\|^2)$,
- neural network: $\kappa(x, x') = \tanh(\alpha \langle x, x' \rangle + \beta)$.

Once the kernel function $\kappa$ is given, methods designed for solving dual problems of linear SVMs can be easily adapted to solve corresponding dual problems of kernel SVMs. But such extensions for methods that is designed to solve primal forms of linear SVMs are not trivial.

Zhang et al. (2012) have proposed a linearization approach for the $L_1$-loss kernel SVM (10), which is briefly reviewed below.

### 2.2 Linearized $L_1$-loss kernel SVM

Define the positive semidefinite kernel matrix $\mathbf{K} \in \mathbb{R}^{(n+m) \times (n+m)}$ as

$$K_{ij} = \langle \psi(x_i), \psi(x_j) \rangle, \; i, j = 1, \ldots, m + n.$$  

Rewrite $\mathbf{K}$ in the following partition

$$\mathbf{K} = \begin{bmatrix} \mathbf{K}_{rr} & \mathbf{K}_{re} \\ \mathbf{K}_{er} & \mathbf{K}_{ee} \end{bmatrix} \quad \text{with} \; \mathbf{K}_{rr} \in \mathbb{S}^n, \; \mathbf{K}_{ee} \in \mathbb{S}^m, \; \mathbf{K}_{re} \in \mathbb{R}^{n \times m}. \quad (8)$$

The following result comes form Proposition 1 in (Zhang et al. 2012), which addresses the method of transforming the $L_1$-loss kernel SVM

$$\begin{align*}
\min_{\mathbf{w}, b} & \quad \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1}^n \xi_i \\
\text{s.t.} & \quad y_i (\mathbf{w}^\top \psi(x_i) + b) \geq 1 - \xi_i, \; \xi_i \geq 0, \; i = 1, \ldots, n.
\end{align*}\quad (9)$$

into the $L_1$-loss linear SVM

$$\begin{align*}
\min_{\mathbf{w}, b} & \quad \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1}^n \xi_i \\
\text{s.t.} & \quad y_i (\mathbf{w}^\top \hat{x}_i + b) \geq 1 - \xi_i, \; \xi_i \geq 0, \; i = 1, \ldots, n.
\end{align*}\quad (10)$$

**Proposition 1** Given the training data $\mathbf{X}_r$, label $\mathbf{y}_r$ and test data $\mathbf{X}_e$ as defined in (3). An $L_1$-loss kernel SVM model (7) trained on $\mathbf{X}_r, \mathbf{y}_r$ and tested on $\mathbf{X}_e$ is equivalent to a linear SVM (10) trained on $\mathbf{F}_r, \mathbf{y}_r$ and tested on $\mathbf{F}_e$, where

$$\mathbf{K} = \begin{bmatrix} \mathbf{F}_r & \mathbf{F}_r \end{bmatrix} \begin{bmatrix} \mathbf{F}_r^\top \\ \mathbf{F}_e^\top \end{bmatrix}, \; \mathbf{F}_r = \begin{bmatrix} \hat{x}_{1r}^T \\ \vdots \\ \hat{x}_{nr}^T \end{bmatrix}, \; \mathbf{F}_e = \begin{bmatrix} \hat{x}_{1e}^T \\ \vdots \\ \hat{x}_{ne}^T \\ \hat{x}_{n+1, e}^T \end{bmatrix} \quad (11)$$

is any decomposition of the positive semidefinite kernel matrix $\mathbf{K}$ evaluated on $(\mathbf{X}_r, \mathbf{X}_e)$, and the factor $\mathbf{F}_r \in \mathbb{R}^{n \times q}$ and $\mathbf{F}_e \in \mathbb{R}^{m \times q}$ can be deemed as "virtual samples" whose dimensionality $q$ is the rank of $\mathbf{K}$. 

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By Proposition 1, Zhang et al. proposed a framework to solve the $L_1$-loss kernel SVM, by solving the $L_1$-loss linear SVM. Note that the linearization process may not be easy, for instance the exact spectral decomposition of the kernel matrix $K$ takes $O(n^3)$ operations. Consequently, an approximation is further conducted by using the Nyström methods \cite{williams2001}, which approximates $F_r \in \mathbb{R}^{n \times q}$ by $\tilde{F}_r \in \mathbb{R}^{n \times k}$. Finally, an $L_1$-loss linear SVM model is trained on $\tilde{F}_r$.

The idea in Proposition 1 provides us a way to make use of fast solvers in linear SVM. As we mentioned in Introduction, one of the latest fast solvers is a semismooth Newton’s method \cite{yin2019} for $L_2$-loss linear SVM

\[
\min_{w, b} \frac{1}{2} \|w\|^2 + C \sum_{i=1}^{n} \max(0, 1 - y_i(x_i^\top w + b))^2. \tag{12}
\]

It is demonstrated by \cite{yin2019} that semismooth Newton’s method is competitive with DCD and TRON in LIBLINEAR. Inspired by Zhang et al. \cite{zhang2012}, we can explore the technique in Proposition 1 and extend semismooth Newton’s method \cite{yin2019} to solve the $L_2$-loss SVM. We state our approach in the following section.

3 A linearization and approximation approach

In this section, we first get the equivalence of the $L_2$-loss kernel SVM and the $L_2$-loss linear SVM with some relationship between their data, similar to the way in Proposition 1. Then we apply the Nyström method \cite{williams2001} to get an approximation of the kernel matrix, based on which a reduced $L_2$-loss linear SVM is obtained.

3.1 Equivalent linear SVM

Similar to Proposition 1, we have following result, whose proof is similar to that of Proposition 1. For consideration of completion, we include our proof in Appendix A.

**Theorem 1** An $L_2$-loss SVM \cite{zhang2012} trained on $X_r$, $y_r$ and tested on $X_e$ is equivalent to a linear $L_2$-loss SVM \cite{yin2019} trained on $F_r$, $y_r$ and tested on $F_e$, where $K$ is defined as in \cite{zhang2012} and $F_r, F_e$ are defined as in \cite{yin2019}.

3.2 Low-rank approximation of the kernel matrix

By Theorem 1 solving $L_2$-loss kernel SVM \cite{zhang2012} is equivalent to solving \cite{yin2019}, and the predicting label for $\hat{x}_i$ is given by

\[
\text{sign}(\hat{x}_i^\top w^* + b^*), \ i = n + 1, \ldots, n + m. \tag{13}
\]

Now the key is to find $F_r, F_e$ such that \cite{yin2019} holds. Since kernel matrix $K_{rr}$ is semidefinite, an obvious way is just to use the spectral decomposition of $K_{rr}$, however the computation cost is high as we mentioned before. Consequently, it is a good choice to approximate the kernel matrix, such as using low-rank approximation. Consider solving the following optimization problem

\[
\min_{M \in \mathbb{S}^n} \frac{1}{2} \|K_{rr} - M\|, \text{ s.t. } \text{rank}(M) \leq k, \ M \text{ is positive semidefinite}, \tag{14}
\]
the solution is denoted as $K^{(k)}_{rr}$. Then
\[
K^{(k)}_{rr} = F^{(k)}_r (F^{(k)}_r)^\top,
\]
where
\[
F^{(k)}_r = U^{(k)}_r (A^{(k)}_r)^{1/2}
\]
and $A^{(k)}_r$ is a diagonal matrix with diagonal entries being top $k$ eigenvalues of $K_{rr}$ and $U^{(k)}_r$ stands for corresponding eigenvectors.

However, it is not applicable when the kernel SVM is trained on a dataset with thousands of data points. In fact, exact computation of the top $k$ eigenvectors requires $O(n^2 k)$ time and $O(n^2)$ space, which could be extremely time consuming. Another popular approximation method, which has been well studied recently, is Nyström method (Williams and Seeger 2001; Kumar et al. 2009). Given a set of training samples $X_r$, a set of testing samples $X_e$ and the kernel matrix $K$ that is defined as in (8), the Nyström method chooses a subset of $k$ samples $L \in \mathbb{R}^{k \times q}$, named landmark points set, from training samples $X_r$ and provides a rank-$k$ approximation of the kernel matrix as
\[
\tilde{K}_{rr} = K_{rl} K_{ll}^{-1} K_{rl}^\top, \quad \tilde{K}_{ee} = K_{el} K_{ll}^{-1} K_{el}^\top,
\]
where $K_{rl}$ is the kernel matrix on $X_r$ and $L$, $K_{el}$ is the kernel matrix on $X_e$ and $L$, $K_{ll}$ is the kernel matrix on $L$ (Williams and Seeger 2001: Eq.(10)). We refer to Williams and Seeger (2001) for more details of Nyström method.

Consequently, assume that the spectral decomposition of $K_{ll}$ is
\[
K_{ll} = V \Lambda V^{-1},
\]
where $K_{ll}$ is positive definite. Let $M = VA^{-\frac{1}{2}}$, referred to as the mapping matrix, then
\[
\tilde{K}_{rr} = K_{rl} V A^{-\frac{1}{2}} (K_{rl} V A^{-\frac{1}{2}})^\top = K_{rl} M (K_{rl} M)^\top.
\]
Similarly we have
\[
\tilde{K}_{ee} = K_{el} M (K_{el} M)^\top.
\]

Denote
\[
\tilde{F}_r = K_{rl} M, \quad \tilde{F}_e = K_{el} M.
\]

Instead of solving $L_2$-loss kernel SVM model (3), we can train the following linear SVM on $\tilde{F}_r$, $y_r$ and test on $\tilde{F}_e$
\[
\begin{align*}
\min_{w, b} & \frac{1}{2} \|w\|^2 + C \sum_{i=1}^t \xi_i^2 \\
\text{s.t.} & \ y_i (w^\top \tilde{x}_i + b) \geq 1 - \xi_i, \ \xi_i \geq 0
\end{align*}
\]
where
\[
\tilde{F}_r := \begin{bmatrix} \tilde{x}_1 \\ \vdots \\ \tilde{x}_n \end{bmatrix}, \quad \tilde{F}_e := \begin{bmatrix} \tilde{x}_{n+1} \\ \vdots \\ \tilde{x}_{n+m} \end{bmatrix}.
\]

Let $(\tilde{w}^*, \tilde{b}^*)$ be the optimal solution of (17), then the predicting label for testing data $x_i$ is
\[
\text{sign}( (\tilde{w}^*)^\top \tilde{x}_i + \tilde{b}^*), \ i \in \{n+1, n+2, \cdots, n+m\}.
\]
We call (17) the reduced $L_2$-loss linear SVM.
4 Error analysis on the approximation of kernel matrices

In this section, we analyze the difference between $w$ obtained by training $L_2$-loss kernel SVM on $X_r = \{x_1, x_2, \ldots, x_n\}$ with kernel matrix being $K_{rr}^{(k)}$ and $\hat{w}$ with $\hat{K}_{rr}$. Here for convenience, we omit the bias term of SVMs.

Denote that $W$ is a set of all the possible $w, \hat{w}$ obtained by solving two problems above. Let $\psi(\cdot), \kappa(\cdot, \cdot)$ be the feature mapping function and the kernel function associated to $K_{rr}^{(k)}$, and $\tilde{\psi}(\cdot), \tilde{\kappa}(\cdot, \cdot)$ associated to $\hat{K}_{rr}$. The hypothesis sets we consider are

$$W = \{ w | \exists w \in W, \forall x \in X_r, h(x) = w^T \psi(x) \}$$

and

$$\hat{W} = \{ \hat{w} | \exists \hat{w} \in \hat{W}, \forall x \in X_r, \hat{h}(x) = \hat{w}^T \tilde{\psi}(x) \}.$$ 

We’ll use the same notation in following passage and Appendix B.

We need the following assumption which is also used in Mohri et al. (2018: Chapter 6, Page 117).

**Assumption 1** Assume that there exist $\rho \geq 0$, $G \geq 0$ such that

$$\max\{\kappa(x, x), \tilde{\kappa}(x, x)\} \leq \rho, \forall x \in X_r,$$

and

$$\max\{|\kappa(x)|, |\tilde{\kappa}(x)|\} \leq G, \forall x \in X_r, \kappa(\cdot) \in H, \forall \tilde{\kappa}(\cdot) \in \hat{H}.$$

Our result is stated as follows, whose proof is in Appendix B.

**Theorem 2** Under Assumption 1 we have

$$\|w - \hat{w}\|^2 \leq 4C^2G(G + 1)\rho^2 \left[ k\epsilon_f^2 + \lambda_1 tr(A) + k e_2 tr(\tilde{A}_{(k)}) \left( e_f^2 + tr(A_{(k)})^2 \right) \right],$$

where $A \in \mathbb{R}^{k \times k}$ is a diagonal matrix with entries

$$A_{ii} = \max\{\frac{1}{A_{ii}} + \frac{1}{A_{ii}^2}, \frac{3}{A_{ii}} - \frac{1}{A_{ii}^2} \},$$

$\Lambda = \text{diag}(\lambda_1, \ldots, \lambda_n)$ and $\tilde{\Lambda} = \text{diag}(\tilde{\lambda}_1, \ldots, \tilde{\lambda}_n)$ are the exact and Nyström approximate eigenvalues (sorted in descending order) of the kernel matrix and

$$e_f = (\sum_{i=k+1}^n \lambda_i^2)^{\frac{1}{2}} + \xi_f,$$

$$e_2 = \lambda_{k+1} + \xi_2,$$

in which $\xi_f$ and $\xi_2$ are known error bounds on the gaps between the Nyström low-rank approximation and the original kernel matrix with following definition

$$\xi_f := \|K_{rr} - \hat{K}_{rr}\|_F,$$

$$\xi_2 := \|K_{rr} - \hat{K}_{rr}\|_2.$$

From this theorem, we can see that $\|w - \hat{w}\|$ is bounded by the gap between the Nyström low-rank approximation and the original kernel matrix. Therefore the smaller the approximation error of kernel matrix, the smaller the $\|w - \hat{w}\|$ is, i.e., the more accurate the $\hat{w}$ is.

Let $(w^*, b^*, y^*_d, h^*_d) = L_2(X_r, y_r, X_c; \psi)$ denote the solution $(w^*, b^*)$ of training $L_2$-loss kernel SVM trained on data $(X_r, y_r)$ with kernel $\psi$, and $y^*_c, h^*_c$ denote the predicting labels and values respectively, for test data $X_c$, i.e., $(h^*_c)_i = w^* \psi(x_{n+i}) + b^*$. Let $I$ be the identity operator. We have similar notations for others. The content in this article has the relations as shown in Fig. I.
\[(\mathbf{w}^\mathcal{X}, b^\mathcal{X}, y^\mathcal{X}_e, h^\mathcal{X}_e) = L_2(F_r, y_r, F_e; \mathcal{I})\]

\[(\mathbf{w}^\kappa, b^\kappa, y^\kappa_e, h^\kappa_e) = L_2(X_r, y_r, X_e; \psi^0)\]

\[y^\mathcal{X}_e = y^\kappa_e, h^\mathcal{X}_e = h^\kappa_e \quad \text{(Theorem 1)}\]

\[(\mathbf{w}, b, y_e, h_e) = L_2(X_r, y_r, X_e; \psi) = L_2(F_r, y_r, F_e; \mathcal{I})\]

\[\|\mathbf{w} - \tilde{\mathbf{w}}\| \quad \text{(Theorem 2)}\]

**Fig. 1** Structure of our article

**Remark:** Zhang et al (2012) also do similar work as in Fig. 1 but for \(L_1\)-loss kernel SVM and corresponding \(L_1\)-loss linear SVM. Another difference of our work from theirs is that we employ the latest highly efficient semismooth Newton’s method to solve the reduced linear SVM.

### 5 Semismooth Newton’s method for the reduced \(L_2\)-loss linear SVM

Next, we will apply semismooth Newton’s method (Yin and Li 2019) to solve the reduced \(L_2\)-loss linear SVM (17), which is equivalent to the following unconstrained problem

\[
\min_{\mathbf{w} \in \mathbb{R}^p, b \in \mathbb{R}} \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1}^n \max(1 - y_i (\mathbf{w}^\top \tilde{x}_i + b), 0)^2.
\]  

(20)

Due to the fact that the bias term \(b\) hardly affect the numerical performance as shown in (Ho and Lin 2012: Section 4.5), we omit the bias term, and solve the following unbiased model (by setting \(\tilde{x}_i \leftarrow [x_i, 1], \tilde{\mathbf{w}}_i \leftarrow [\mathbf{w}_i, 1]\))

\[
\min_{\mathbf{w} \in \mathbb{R}^p} \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1}^n \max(1 - y_i \mathbf{w}^\top \tilde{x}_i, 0)^2 := f(\mathbf{w}).
\]  

(21)

At iteration \(j\), let \(I_j := \{i : 1 - y_i \tilde{x}_i^\top \mathbf{w}_j > 0\}\) and denote

\[\tilde{\partial}^2 f(\mathbf{w}^j) = \{I + 2C \sum_{i \in I_j} \tilde{x}_i \tilde{x}_i^\top\}.
\]

Details of the semismooth Newton’s method are given in Alg. 1.

The advantage of this semismooth Newton’s method is that it enjoys global convergence and quadratic convergence rate, as we show in the following theorem.
Algorithm 1: A globalized semismooth Newton’s method for (21)

1. Given $j = 0$. Choose $w^0, \sigma \in (0,1), \rho \in (0,1), \delta > 0$ and $\eta_0 > 0, \eta_1 > 0$;
2. Calculate $\nabla f(w^j)$. If $\|\nabla f(w^j)\| \leq \delta$, stop. Otherwise go to step 3;
3. Select an element $V^j \in \hat{\partial}^2 f(w^j)$ and apply Conjugate Gradient (CG) method [Hestenes and Stiefel 1952] to find an approximate solution $d^j$ by
   \[ V^j d^j + \nabla f(w^j) = 0 \]
   such that
   \[ \|V^j d^j + \nabla f(w^j)\| \leq \mu_j \|\nabla f(w^j)\| \]
   where $\mu_j = \min(\eta_0, \eta_1 \|\nabla f(w^j)\|);$
4. Do line search to find the smallest positive integer $m_j$ such that the following holds
   \[ f(w^j + \rho m_j d^j) \leq f(w^j) + \sigma \rho m_j \nabla f(w^j)^\top d^j. \]
   Let $\alpha_j = \rho m_j$;
5. Let $w^{j+1} = w^j + \alpha_j d^j$, $j = j + 1$. Go to step 2;

Remark As analyzed by Yin and Li (2019), the main computational cost in each iterations of semismooth Newton’s method lies in Step 3 of Alg. 1 which is to calculate $V^j h$, for any $h \in \mathbb{R}^p$. By exploring the sparse structure of the optimal solution of (21), the computational cost of computing $V^j h$ can be reduced to $O(n|I_j|)$, where $|I_j|$ is the number of elements in the set $I_j$ and $|I_j| \ll n$.

Theorem 3 (Yin and Li 2019: Theorem 1) Let $w^*$ be a solution of (20). Then every sequence generated by (11) is quadratically convergent to $w^*$.

Now we summarize our Semismooth-Newton’s-method-based Linearization and Approximation approach (LASN) as follows. Firstly, we choose $k$ landmark points by k-means clustering algorithm, then use Nyström approximation to get $\tilde{K}_{ll}$. Then we get $\tilde{F}_r$, and train linear SVM by semismooth Newton’s method. The details of our approach is given in Alg. 2 and the predicting process are given in Alg. 3.

In Alg. 2 the first four steps take $O(nkp + k^3 + nk^2)$ operations, where $k$ is usually between $n/10$ and $n/100$.

Algorithm 2: LASN Training stage

1. Choose $k$ landmark points $L$ by efficient k-means method and then compute $K_{ll}$ and $K_{rl}$;
2. Compute spectral decomposition of $K_{ll}$ to get $V, A$ such that $K_{ll} = VAV^{-1}$;
3. Compute $\Lambda^{-\frac{1}{2}}$ and then the mapping matrix $M = V \Lambda^{-\frac{1}{2}}$;
4. Compute $K_{rM}$;
5. Train $L_2$-loss linear SVM on $K_{rM}$ by semismooth Newton’s method;
Algorithm 3: LASN Predicting stage

**Input:** testing data $X_e$, weight vector $\hat{w}$, mapping matrix $M$
**Output:** predicting label $\hat{y}_e$

1. Compute $K_{er}$;
2. Predict by $\hat{y}_e = \text{sign}(K_{er} M \hat{w})$;

6 Numerical result

In this section, we conduct extensive numerical test to verify the efficiency of our method. It is divided into three parts. In the first part, we analyze how to choose landmark set size $k$ and cost parameter $C$ for the proposed method. Then we compare numerical results of low-rank linearized method with different linear SVMs’ solvers. Finally, we compare the performance of our algorithm and the solver in LIBSVM.

All experiments are tested in Matlab R2018b in Windows 10 on a Microsoft Surface Pro 4 with an Intel(R) Core(TM) i5-6300U CPU at 2.40 GHz, 2.50 GHz and of 8 GB RAM. Throughout the experiment, we use the Gaussian kernel $\kappa(x, y) = \exp(-\|x - y\|^2/\gamma)$ where $\gamma$ is chosen as the average squared distance between data points of each dataset (Kumar et al. 2009).

We use standard real datasets available at LIBSVM site^[1]. Due to the need of computing kernel matrix and sampling with k-means method, our algorithm is hard to tackle with dataset with millions of instance or each instance having millions of features on limited computing resources (eg. PC) and lose it is efficiency. Therefore we screen out those datasets with $p \times n > 10^{10}$. For datasets without explicitly splitting into training set and testing set, we use the first 60% data points as training set and the other 40% as testing set.

Implementations In Step 1 of Alg. 2 we adopted a fast approximate k-means sampling method using only a few iterations, which does not necessarily converge. Then we use the center obtained from the k-means method as landmark points. In the fast k-means sampling procedure, if one particular dataset has more than 20000 data points, for efficiency we only use the first 20000 data points to choose landmark points. In Step 4 of Alg. 2 let $A = \text{diag}(a_1, a_2, \cdots, a_k)$, we set $a_i = 0$ if $a_i < 10^{-6}$ then compute the inverse of $A$. We improve the efficiency of this algorithm by computing the distance between data points in advance and using it in following multiple steps.

6.1 Choosing parameters

In this part, we analyze the impact of different choices of landmark set size $k$ and the cost parameter $C$. For each dataset we randomly choose 80% data points of original training set for training and the other 20% of training set for cross-validation, so we are going to report two accuracies: accuracy of predicting on the cross-validation set (CV accuracy) and accuracy of predicting on the testing set (testing accuracy).

6.1.1 Landmark set size $k$

From the theoretical point of view, the larger $k$ is, the more accurate the approximation of the kernel matrix is. However, recall that $n$ is the number of training data points, $k$ must satisfy $k \leq n$. On

[^1]: https://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/
the other hand, $k$ is also the dimension of the transformed linear data points, which means that the SVM is going to be trained on data with dimensions of $n \times k$. Consequently, for efficiency and saving computing resources, $k$ shouldn’t be too large.

We test on the datasets reported in Table 1. According to size of these datasets, we choose $k = \{50, 100, 200, 500, 1000\}$ with corresponding $\log(k) = \{1.7, 2.0, 2.3, 2.7, 3.0\}$. Here we set cost parameter $C = 10$. Recall the notation for number of features is $p$ and the one for number of instance is $n$. The datasets can be divided into three groups: Large Datasets (LD) with $p \times n > 10^8$, Medium Datasets (MD) with $10^6 < p \times n < 10^8$ and Small Datasets (SD) with $p \times n < 10^6$.

Table 1 Groups of datasets

| Dataset name | number of instance $n$ | number of features $p$ | kernel parameter $\gamma$ | Group   |
|--------------|-----------------------|------------------------|---------------------------|---------|
| skin_nonskin | 42244                 | 3                      | 4843.688                  | SD      |
| a2a          | 1812                  | 123                    | 7.6484                    | SD      |
| ijcnn        | 39992                 | 22                     | 1.2974                    | SD      |
| cod-rna      | 47628                 | 8                      | 36592.4                   | MD      |
| a9a          | 26048                 | 123                    | 7.6723                    | MD      |
| gisette_scale| 4800                  | 5000                   | 1287.527                  | MD      |
| rcv1_binary  | 16193                 | 47236                  | 0.98094                   | LD      |
| news20_binary| 9597                  | 1355191                | 0.94151                   | LD      |
| real-sim     | 34708                 | 20958                  | 0.98791                   | LD      |

- Large datasets

[Fig. 2] Results of LASN on large datasets with different $k$’s

As showed in Fig. 2, for this group of datasets, larger $k$ usually means higher predicting accuracy but longer training time too. There is a tradeoff between training time and predicting accuracy. Letting $k = \sqrt{n}$ could be a good choice.

- Medium datasets

In Fig. 3 for this group of datasets, letting $k = \sqrt{n}$ again could be a good choice, since larger $k$ won’t significantly improve predicting accuracy and it makes the training process consume more time.
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Fig. 3 Results of LASN on medium datasets with different k’s

- Small datasets

Fig. 4 Results of LASN on small datasets with different k’s

From Fig. 4, for small datasets, using $k = \sqrt{n}$ could be a good choice too. However, increasing $k$ can bring different outcomes, which can be related to the nature of each unique dataset. Luckily, the training time on this group of datasets are short no matter how large $k$ is. We can try several $k$’s around $\sqrt{n}$ to find out the best choice.

In all the figures above, we can see that generally the training time of our algorithm increase linearly with the number of landmark points. It means that our algorithm is scalable through adjusting the parameter $k$.

6.1.2 Cost parameter $C$

According to the results above, we have chosen the landmark point size $k$ for each dataset. Now we are going to explore proper choice of the cost parameter $C$ given the chosen $k$ of each dataset. Fig. 5 and Fig. 6 displays the testing accuracy, CV accuracy and the time of training on several datasets with fixed $k$ and different $C$’s ranging from $10^{-4}$ to $10^4$.

In Fig. 5, the training time of our algorithm increase as $C$ becomes larger in an accelerated speed and increase significantly from $C = 10$ to $C = 100$. For each dataset, accuracy generally increase as $C$ becomes larger and comes to be stable when $C = 10$. In Fig. 6, we have similar results to that in Fig. 5. However, training time is unstable as $C$ increases and the range of training time is small for all datasets except real_sim.

To conclude, $C$ being 10 is usually a good choice, with which our algorithm usually can get a good accuracy of predicting without using too much time.

Fig. 5 Results of LASN on small datasets with different k’s
6.2 Numerical comparisons between different linear solvers

One important step in our algorithm is Step 5, which is to solve the reduced linear SVM with semismooth Newton’s method. In this part, as comparisons, we use two solvers in liblinear, which are the dual coordinate descent method (DCD) (Hsieh et al. 2008) and the trust region Newton method (TRON) (Lin et al. 2008), and compare the numerical results with our algorithm. For the three resulting algorithms, denoted as LA-SN (Alg. 2 with semismooth Newton’s method as subsolver), LA-DCD (Alg. 2 with DCD as subsolver) and LA-TRON (Alg. 2 with TRON as subsolver), we’ll use the same cost parameter $C = 10$ the number of landmark points $k$ for each dataset. For each dataset, we repeat each algorithm for ten times, and report the mean of the time used for solving the reduced linear SVM (denoted by $t_{\text{linear}}$) and predicting accuracies.

In Table 2, we can see that the three algorithms have similar performance in predicting accuracies, but the semismooth Newton’s method costs much less time than DCD and TRON in training the reduced linear SVM. It verifies that the semismooth Newton’s method is a good choice for the linearization and approximation approach.

6.3 Numerical comparisons with LIBSVM

In this part, we compare our algorithm with LIBSVM (Chang and Lin 2011). For both algorithms, we’ll use the same cost parameter $C = 10$. Since the results of LASN are non-deterministic, for each dataset we repeat LASN for ten times and then report mean and standard deviation of training time and predicting accuracies on testing set.

As can be seen in Table 3, with proper choice of $k$, LASN outperforms LIBSVM in terms of both training time and predicting accuracy on majority of the datasets (marked in bold). Especially for w8a, a9a and real-sim datasets (marked in red), we can clearly see our algorithm has great advancement in training speed while keeping good predicting accuracy. It should be noticed that $k$ can be chosen in
Table 2 Information of datasets used in Subsection 6.2 and Subsection 6.3

| Dataset name | number of instance n | number of features p |
|--------------|----------------------|----------------------|
| ijcnn        | 49990                | 23                   |
| w1a          | 2477                 | 300                  |
| w2a          | 3470                 | 300                  |
| w3a          | 2990                 | 300                  |
| w4a          | 3618                 | 300                  |
| w5a          | 9888                 | 300                  |
| w6a          | 17188                | 300                  |
| w7a          | 13961                | 300                  |
| w8a          | 43735                | 300                  |
| phishing     | 2962                 | 67                   |
| mushrooms    | 4874                 | 112                  |
| real-sim     | 43385                | 20958                |
| skin_nonskin | 52806                | 3                    |
| cod-rna      | 59535                | 8                    |
| madelon      | 323                  | 500                  |
| liver-disorders | 145            | 5                    |
| a1a          | 1605                 | 123                  |
| a2a          | 2265                 | 123                  |
| a3a          | 3185                 | 123                  |
| a4a          | 4781                 | 123                  |
| a5a          | 6414                 | 123                  |
| a6a          | 6414                 | 123                  |
| a7a          | 6414                 | 123                  |
| a8a          | 3318                 | 123                  |
| a9a          | 32561                | 123                  |
| rcv1_binary  | 20242                | 47236                |
| news20_binary| 11997                | 1355191              |
| gisette_scale| 6000                 | 5000                 |
| Dataset          | LA-SN$^1$ $t_{linear}(s)$ | LA-SN$^1$ accuracy(%) | LA-DCD$^1$ $t_{linear}(s)$ | LA-DCD$^1$ accuracy(%) | LA-TRON$^1$ $t_{linear}(s)$ | LA-TRON$^1$ accuracy(%) |
|------------------|---------------------------|------------------------|-----------------------------|-------------------------|------------------------------|--------------------------|
| ijcnn            | 11.6998                   | 98.9363                | 15.6948                     | 98.94                   | 14.2318                      | 98.94                    |
| w1a              | 0.0454                    | 97.5478                | 0.1234                      | 97.5491                 | 0.125                        | 97.5491                  |
| w2a              | 0.079                     | 97.6516                | 0.188                       | 97.6521                 | 0.192                        | 97.6521                  |
| w3a              | 0.077                     | 97.7523                | 0.1664                      | 97.7501                 | 0.1738                       | 97.7501                  |
| w4a              | 0.0938                    | 97.8444                | 0.2222                      | 97.8388                 | 0.2254                       | 97.8388                  |
| w5a              | 1.4526                    | 98.2755                | 2.2548                      | 98.2755                 | 2.2618                       | 98.2755                  |
| w6a              | 2.3096                    | 98.5332                | 4.1908                      | 98.5332                 | 4.216                        | 98.5332                  |
| w7a              | 2.1148                    | 98.576                 | 3.4694                      | 98.5752                 | 3.4396                       | 98.5752                  |
| w8a              | 5.9344                    | 98.7947                | 10.9314                     | 98.7934                 | 10.9452                      | 98.7934                  |
| phishing         | 0.0236                    | 95.4453                | 0.0686                      | 95.3846                 | 0.074                        | 95.3846                  |
| mushrooms        | 0.084                     | 95.343                 | 0.121                       | 95.3553                 | 0.1274                       | 95.3553                  |
| real-sim         | 8.2336                    | 81.4126                | 13.7686                     | 81.4361                 | 13.7766                      | 81.4361                  |
| skin nonskin     | 0.1554                    | 94.2093                | 0.6256                      | 94.1946                 | 0.603                        | 94.1946                  |
| cod-rna          | 0.2664                    | 89.2636                | 5.3674                      | 89.2601                 | 5.3562                       | 89.2601                  |
| madelon          | 0.0178                    | 62                     | 0.009                       | 61.6667                 | 0.0118                       | 61.6667                  |
| liver-disorders  | 0.006                     | 58.8                   | 0.0082                      | 58.5                    | 0.0096                       | 58.5                     |
| a1a              | 0.0362                    | 83.5883                | 0.1006                      | 83.5793                 | 0.1034                       | 83.5793                  |
| a2a              | 0.0566                    | 83.648                 | 0.1666                      | 83.6044                 | 0.1632                       | 83.6044                  |
| a3a              | 0.1006                    | 84.04                  | 0.2388                      | 84.0298                 | 0.2412                       | 84.0298                  |
| a4a              | 0.157                     | 84.3549                | 0.3688                      | 84.3585                 | 0.377                        | 84.3585                  |
| a5a              | 0.204                     | 84.4877                | 0.512                       | 84.4862                 | 0.509                         | 84.4862                  |
| a6a              | 0.1938                    | 84.4637                | 0.5084                      | 84.4581                 | 0.5162                       | 84.4581                  |
| a7a              | 0.2064                    | 84.4991                | 0.5106                      | 84.4858                 | 0.5122                       | 84.4858                  |
| a8a              | 0.106                     | 84.2636                | 0.2458                      | 84.2534                 | 0.2526                       | 84.2534                  |
| a9a              | 0.6758                    | 85.0709                | 3.5074                      | 85.0562                 | 3.518                         | 85.0562                  |
| rcv1_binary      | 2.421                     | 95.7131                | 4.0992                      | 95.7131                 | 4.0766                       | 95.7131                  |
| news20_binary    | 2.1738                    | 73.31                  | 3.49                         | 73.3075                 | 3.5296                       | 73.3075                  |
| gisette_scale    | 0.0564                    | 97.56                  | 0.141                        | 97.56                   | 0.1426                       | 97.56                    |
| Dataset         | LIBSVM($L_2$-loss) | LASN  |
|-----------------|---------------------|-------|
|                 | $t$(s)  | accuracy(%) | $t$(s)  | accuracy(%) | k     |
| ijcnn           | 127.46   | 98.98       | 72.98   | 99.07(0.02) | 3000  |
| w1a             | 0.86     | 97.24       | 0.80    | 97.55(0.11) | 200   |
| w2a             | 1.70     | 97.32       | 0.92    | 97.62(0.10) | 200   |
| w3a             | 1.25     | 97.34       | 0.77    | 97.82(0.12) | 200   |
| w4a             | 1.73     | 97.41       | 0.92    | 97.88(0.07) | 200   |
| w5a             | 43.58    | 97.46       | 2.33    | 97.70(0.08) | 200   |
| w6a             | 136.57   | 97.60       | 4.09    | 97.94(0.11) | 200   |
| w7a             | 90.36    | 97.66       | 4.33    | 98.04(0.08) | 200   |
| w8a             | 819.98   | **99.45**   | **7.58**| 98.11(0.08) | 200   |
| phishing        | 0.67     | **98.08**   | 0.96    | 96.99(0.16) | 200   |
| mushrooms       | 4.37     | 38.39       | 1.71    | 95.66(2.81) | 200   |
| real-sim        | 921.20   | 76.54       | **119.61**(34.83) | 81.03(1.12) | 1000  |
| skin, nonskin   | 119.12   | 32.54       | 20.08   | 93.57(0.24) | 1000  |
| cod-rna         | 344.82   | **92.35**   | 21.29   | 89.65(0.03) | 1000  |
| madelon         | 0.11     | 50.00       | 8.36    | 62.00(0.00) | 323   |
| liver-disorders | 0.00     | 50.00       | 0.03    | 58.50(0.00) | 145   |
| a1a             | 0.51     | 76.50       | 0.49    | 83.61(0.14) | 200   |
| a2a             | 1.13     | 76.89       | 0.71    | 83.56(0.11) | 200   |
| a3a             | 1.88     | 77.26       | 1.04    | 84.00(0.08) | 200   |
| a4a             | 3.90     | 78.05       | 1.34    | 84.34(0.15) | 200   |
| a5a             | 18.05    | 78.33       | 2.17    | 84.47(0.08) | 200   |
| a6a             | 18.08    | 78.19       | 1.71    | 84.40(0.10) | 200   |
| a7a             | 18.13    | 78.51       | 1.71    | 84.54(0.10) | 200   |
| a8a             | 1.85     | 77.66       | 1.34    | 84.22(0.17) | 200   |
| a9a             | 679.82   | 80.65       | **7.44**| **85.03**(0.07) | 200   |
| rcv1_binary     | 573.22   | **96.60**   | **173.02**(0.54) | 95.74(0.03) | 1000  |
| news20_binary   | 637.20   | **74.90**   | **444.03**(4.25) | 73.52(0.10) | 1000  |
| gisette_scale   | 132.50   | **98.00**   | **54.43**(0.85) | 97.66(0.18) | 100   |
a different way according to the user’s need, our algorithm is scalable so that it can achieve greater training speed at the cost of predicting accuracy.

7 Conclusions

In this paper, we proposed a new approach to deal with the kernel SVMs. After linearizing the kernel matrix and approximating it by Nyström methods, we solve the reduced linear SVM by the highly efficient semismooth Newton’s method. We also provide theoretical guarantee for the new approach. Extensive numerical results demonstrate the efficiency of the proposed approach as well as the improvement over the existing state-of-the-art methods.
8 Declarations

This is the section for declarations.

**Funding** Dr. Li’s research was supported by the National Natural Science Foundation of China (No.11671036).

**Conflicts of interest/Competing interests** Not applicable.

**Availability of data and material** All the datasets we use are available at LIBSVM site[2].

**Code availability** We use custom code written by ourself, LIBLINEAR available at LIBLINEAR site[3] and LIBSVM available at LIBSVM site[4].

## Appendices

### A Proof of Theorem 1

**Proof** Recall the kernel $L_2$-loss SVM model[1]. Let $(w^*, b^*)$ be the optimal solution of (1), then predicting label for any $x \in X_e$ is given by (3). Denote

$$
F = \begin{bmatrix}
F_r \\
F_e
\end{bmatrix} = 
\begin{bmatrix}
\hat{x}_1^T \\
\vdots \\
\hat{x}_{n+m}^T
\end{bmatrix}.
$$

The $L_2$-loss SVM model to train $(F_r, y_r)$ is

$$
\min_{w, b} \frac{1}{2} \|w\|^2 + C \sum_{i=1}^{n} \max(1 - y_i(w^T \hat{x}_i + b), 0)^2. \tag{22}
$$

Let $(\hat{w}^*, \hat{b}^*)$ be the optimal solution of (22), then the predicting label for any $\hat{x} \in F_e$ is

$$
sign((\hat{w}^*)^T \hat{x} + \hat{b}^*).$$

To prove our theorem, we only to show that the dual problem of (1) and the dual problem of (22) are equivalent and so are their predicting labels.

Let $A := [-y_1\psi(x_1), \cdots, -y_n\psi(x_n)]$ and $e \in \mathbb{R}^n$ be a vector of all ones. We rewrite (1) equivalently as

$$
\min_{w, \xi, b} \frac{1}{2} \|w\|^2 + C||\xi||^2 \\
\text{s.t.} \quad \xi \geq 0, \\
\quad \xi \geq Aw - by + e. \tag{23}
$$

The corresponding Lagrange function is

$$
L(w, \xi, b, \lambda, \mu) = \frac{1}{2} \|w\|^2 + C||\xi||^2 - \langle \xi, \mu \rangle - \langle \lambda, \xi - Aw + by - e \rangle.
$$

The KKT condition of problem (23) is

$$
\begin{align*}
\nabla_w L(w, \xi; b, \lambda, \mu) &= w + A^T \lambda = 0 \\
\nabla_\xi L(w, \xi; b, \lambda, \mu) &= y^T \lambda = 0 \\
\n\nabla_\lambda L(w, \xi; b, \lambda, \mu) &= 2C \xi - \mu - \lambda = 0 \\
\n\mu^T \xi &= 0, \lambda^T (\xi - Aw + by - e) = 0 \\
\xi &\geq 0, \xi - Aw + by - e \geq 0 \\
\mu &\geq 0, \lambda \geq 0
\end{align*} \tag{24}
$$

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[1] https://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/
[2] https://www.csie.ntu.edu.tw/~cjlin/liblinear/
[3] https://www.csie.ntu.edu.tw/~cjlin/libsvm/
The dual problem of (23) is
\[
\sup_{\lambda \geq 0, \mu \geq 0} \inf_{\xi, b} \left[ \frac{1}{2} \|w\|^2 + \langle A^\top \lambda, w \rangle \right] + \inf_{\xi} \left( C \|\xi\|^2 - \langle \xi, \mu + \lambda \rangle \right) + \inf_{b} \left( (-\lambda^\top y)b + \langle \lambda, e \rangle \right)
\]
which is equivalent to
\[
\min_{\lambda} \frac{1}{2} \|A^\top \lambda\|^2 + \frac{1}{2\eta} \|\lambda\|^2 - \lambda^\top e \\
\text{s.t.} \quad \lambda \geq 0, \quad \lambda^\top y = 0. \tag{25}
\]
Similarly we can derive the dual problem of (23) as
\[
\min_{\lambda} \frac{1}{2} \|\hat{A}^\top \lambda\|^2 + \frac{1}{2\eta} \|\lambda\|^2 - \lambda^\top e \\
\text{s.t.} \quad \lambda \geq 0, \quad \lambda^\top y = 0, \tag{26}
\]
where $\hat{A}^\top := [-y_1 \hat{x}_1, \ldots, -y_n \hat{x}_n]$.

By (25), we have
\[
K_{ij} = \langle \psi(x_i), \psi(x_j) \rangle = \langle \hat{x}_i, \hat{x}_j \rangle, \quad \forall i, j = 1, \ldots, m + n,
\]
which means
\[
A A^\top = \begin{bmatrix}
    y_1^2 \psi(x_1)\top \hat{x}_1 & \cdots & y_1 y_n \psi(x_1)\top \hat{x}_n \\
    \vdots & \ddots & \vdots \\
    y_n y_1 \psi(x_n)\top \hat{x}_1 & \cdots & y_n^2 \psi(x_n)\top \hat{x}_n
\end{bmatrix}
= \begin{bmatrix}
    y_1^2 \hat{x}_1\top \hat{x}_1 & \cdots & y_1 y_n \hat{x}_1\top \hat{x}_n \\
    \vdots & \ddots & \vdots \\
    y_n y_1 \hat{x}_n\top \hat{x}_1 & \cdots & y_n^2 \hat{x}_n\top \hat{x}_n
\end{bmatrix}
= \hat{A} \hat{A}^\top
\]
and then
\[
\frac{1}{2} \|A^\top \lambda\|^2 = \frac{1}{2} \|\hat{A}^\top \lambda\|^2, \quad \forall \lambda.
\]
Therefore problem (25) and problem (26) are equivalent.

Let $\lambda^*$ be the optimal solution of both problem (23) and problem (26), then by KKT condition we have
\[
w^* = A^\top \lambda^*, \quad \hat{w}^* = \hat{A}^\top \lambda^*.
\]
and for any $\lambda^*_i \in (0, 2C)$,
\[
b^* = \frac{1}{y_i} \left( - \frac{1}{2\eta} \lambda^*_i - y_i \psi(x_i)\top w^* + 1 \right)
= - \frac{1}{2\eta y_i} \lambda^*_i - \sum_{j=1}^{n} y_j \psi(x_i)\top \psi(x_j) + \frac{1}{y_i}
= - \frac{1}{2\eta y_i} \lambda^*_i - \sum_{j=1}^{n} y_j \hat{x}_j\top \hat{x}_j + \frac{1}{y_i}
= \hat{b}^*.
\]
Hence for any $x_i \in X$ and corresponding $\hat{x}_i \in F$ we can write
\[
sign((w^*)\top \psi(x_i) + b^*) = \text{sign}((A^\top \lambda^*)\top \psi(x_i) + b^*)
= \text{sign}(- \sum_{j=1}^{n} \lambda^*_j y_j \psi(x_j)\top \psi(x_i) + b^*)
= \text{sign}(- \sum_{j=1}^{n} \lambda^*_j y_j \hat{x}_j\top \hat{x}_i + b^*)
= \text{sign}(- \sum_{j=1}^{n} \lambda^*_j y_j \hat{x}_j\top \hat{x}_i + \hat{b}^*)
= \text{sign}((\hat{A}^\top \lambda^*)\top \psi(x_i) + \hat{b}^*)
= \text{sign}((\hat{w}^*)\top \hat{x}_i + \hat{b}^*).
\]
i.e. the predicting label in (4) and (22) are identical.

B Proof of Theorem 2

Previous studies [Drineas and Mahoney 2006; Cortes et al. 2010; Zhang et al. 2012] have given the bound of error of Nyström approximation, we present it in following lemma.

Lemma 1 Let $F_r^{(k)}$ and $\tilde{F}_r$ be in (13) and (12) respectively. We have

$$\|F_r^{(k)} - \tilde{F}_r\| \leq k e^\frac{1}{2} + \lambda_1 tr(A) + ke_2 tr(\tilde{A}_{(k)}^{-1}) \left( e^\frac{1}{2} + tr(A_{(k)}^2)\right)^\frac{1}{2},$$

(27)

where $A \in \mathbb{R}^{k \times k}$, $A$ and $\tilde{A}$ are defined as in Theorem 2.

We also need the following two lemmas, which are from [Cortes et al. 2010].

Lemma 2 When training the kernel SVM (3) on $X_r$ with kernels $\psi$ and $\tilde{\psi}$ respectively, there is

$$\|w - \tilde{w}\|^2 \leq C_0 \sum_{i=1}^n \left( \left| L(y_i w^T \psi(x_i)) - L(y_i \tilde{w}^T \tilde{\psi}(x_i)) \right| + \left( L(y_i w^T \tilde{\psi}(x_i)) - L(y_i \tilde{w}^T \psi(x_i)) \right) \right),$$

where $L(\cdot)$ is a loss function.

Lemma 3

$$\|\tilde{\psi}(x) - \psi(x)\| \leq \|F_r^{(k)} - \tilde{F}_r\|, \forall x \in X_r.$$
Weight vector $\mathbf{w}$ can be written in terms of dual variables: $\mathbf{w} = \sum_{i=1}^{n} y_i \psi(\mathbf{x}_i) \lambda_i$ where $\lambda_i$ is the dual variable. By the KKT condition, which is similar to (24), we have $2C\xi_i = \lambda_i$ and $\lambda_i (\xi_i + y_i \mathbf{w}^T \psi(\mathbf{x}_i) - 1) = 0, \forall i$. Then we get $\lambda_i$ is either 0 or $2 \frac{C}{n} (1 - y_i \mathbf{w}^T \psi(\mathbf{x}_i))$. Hence

$$\|\mathbf{w}\| = \| \sum_{i=1}^{n} y_i \psi(\mathbf{x}_i) \lambda_i \|$$
$$\leq \sum_{i=1}^{n} |y_i| \| \psi(\mathbf{x}_i) \| |\lambda_i|$$
$$= \sum_{i=1}^{n} \| \psi(\mathbf{x}_i) \| |\lambda_i|$$
$$\leq 2 \frac{C}{n} \sum_{i=1}^{n} \| \psi(\mathbf{x}_i) \| (|\mathbf{w}^T \psi(\mathbf{x}_i)| + 1)$$
$$\leq 2 \frac{C}{n} (G + 1) \sum_{i=1}^{n} \| \psi(\mathbf{x}_i) \|$$

Due to (10) in Assumption 1, there is

$$\text{max}\{\|\psi(\mathbf{x})\|, \|\tilde{\psi}(\mathbf{x})\|\} = \text{max}\{\kappa(\mathbf{x}, \cdot), \tilde{\kappa}(\mathbf{x}, \cdot)\}\sqrt{\max\{\kappa(\mathbf{x}, \mathbf{x}), \tilde{\kappa}(\mathbf{x}, \mathbf{x})\}} \leq \rho \frac{\sqrt{\kappa}}{\sqrt{n}}, \forall \mathbf{x} \in \mathbf{X}.$$

Then

$$\|\mathbf{w}\| \leq 2C\rho G (G + 1) \frac{1}{n} \sum_{i=1}^{n} \| \psi(\mathbf{x}_i) \| \leq 2C\rho G (G + 1) \frac{1}{n},$$

similarly we have

$$\|\tilde{\mathbf{w}}\| \leq 2C\rho G (G + 1) \frac{1}{n} \sum_{i=1}^{n} \| \psi(\mathbf{x}_i) \| \leq 2C\rho G (G + 1) \frac{1}{n}.$$}

Additionally, with Lemma 2 we can get

$$\|\mathbf{w} - \tilde{\mathbf{w}}\|^2 \leq 2C\rho G (G + 1) \frac{1}{n} \sum_{i=1}^{n} \left( \| \psi(\mathbf{x}_i) - \tilde{\psi}(\mathbf{x}_i) \| + \| \tilde{\psi}(\mathbf{x}_i) - \psi(\mathbf{x}_i) \| \right)$$
$$\leq 4C\rho G (G + 1) \frac{1}{n} \sum_{i=1}^{n} \left( \| \psi(\mathbf{x}_i) - \tilde{\psi}(\mathbf{x}_i) \| + \| \tilde{\psi}(\mathbf{x}_i) - \psi(\mathbf{x}_i) \| \right)$$
$$\leq 4C\rho G (G + 1) \frac{1}{n} \| \mathbf{F}_k - \mathbf{F}_r \|,$$

which is desired result.

**Proof of Theorem 2** Combining Lemma 1 and Proposition 2 we have

$$\|\mathbf{w} - \tilde{\mathbf{w}}\|^2 \leq 4C\rho G (G + 1) \frac{1}{n} \left[ k e_1^2 + \lambda_1 tr(\mathbf{A}) + ke_2 tr(\tilde{\mathbf{A}}) \left( e_1^2 + tr(\mathbf{A}^2) \right) \right],$$

which gives the bound of $\|\mathbf{w} - \tilde{\mathbf{w}}\|$. The proof is finished. \(\square\)

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