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# A safe screening rule for Laplacian support vector machine

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#### ABSTRACT

Laplacian support vector machine (LapSVM) has received much concern in semi-supervised learning (SSL) field. To further improve its computational speed, many efficient algorithms have been developed. However, they just focus on the method of solving optimization problem not the scale of the problem itself. Inspired by the sparsity of LapSVM, in this paper, an efficient safe screening rule for LapSVM (SSR-LapSVM) is proposed to address this issue. The proposed method could significantly accelerate the original LapSVM. Through the rule, most of the training samples can be eliminated before solving optimization problem without sacrificing the optimal solution. An important advantage is the safety, in the sense that the solution is exactly the same as the original LapSVM. Different from most existing methods, our approach can effectively deal with the multiple parameter problems. Experiments on both 3 artificial datasets and 24 real world benchmark datasets demonstrate its feasibility and efficiency.

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# 1. Introduction

Since support vector machine (SVM) was proposed by Vapnik (1998), it has been widely applied and well studied (Cortes and Vapnik, 1995; Platt and John, 1999; Steinwart and Christmann, 2008). It has many advantages. Firstly, SVM solves a quadratic programming problem (QPP), which guarantees to obtain the unique solution. Secondly, SVM implements the structural risk minimization principle rather than the empirical risk minimization principle, which can minimize the upper bound of the generalization error.

The traditional SVM is a supervised method which needs the label of each instance for establishing the model (Hu et al., 2013). However, in many real situations, the acquisition of class labels is costly and difficult. Semi-supervised learning (SSL) is a category of learning tasks that also make use of unlabeled data for training (Altınel et al., 2017). In the last decades, SSL has attracted a notable attention (Chapelle et al., 2006; Li et al., 2010) and has been introduced into the SVM to improve its prediction performance. Specifically, Laplacian support vector machine (LapSVM) for SSL has been proposed by Chova et al. (2008), which introduces an additional regularization term on the geometry of both labeled and unlabeled samples (Belkin et al., 2006; Zhu, 2005, 2008). This method has been demonstrated to yield an excellent performance. The model is built on manifold assumption which is suitable for most cases. Its solution characterized by a convex quadratic optimization problem is guaranteed to be globally optimal. By contrast, in most other semi-supervised SVMs (Chapelle et al., 2008; Yang et al., 2014), it needs to solve complex non-convex problems, and the solutions are locally optimal.

Many improvements for LapSVM have been presented to enhance its computational speed and prediction accuracy. In the literature (Melacci and Belkin, 2011), two strategies were presented to solve the primal problem of LapSVM in order to reduce the training time. Qi et al. (2014) proposed a fast LapSVM (FLapSVM) in which authors modify the model of LapSVM to avoid extra matrix and reduce the computation. However, these algorithms just focus on the methods of solving optimization problem not the scale of the problem itself. In addition, the Laplacian graph approaches have been successfully introduced into twin support vector machines (TSVMs) (Jayadeva et al., 2007; Xu et al., 2016, 2017; Xu, 2017; Qi et al., 2012; Yang and Xu, 2016). However, it is still challenging to deal with large datasets on account of the burden of computational cost and memory.

In general, the methods mentioned above make use of both labeled and unlabeled samples to construct more reasonable classifiers. However, compared with the traditional SVM, it takes more computational costs to construct the model. The memory consumption becomes heavy as the scale of data increases. This puts a high demand on the configuration of computers. How to improve the computational speed is a valuable topic.

Recently, a promising sample selection approach called "screening" (Ogawa et al., 2013; Wang et al., 2014; Liu et al., 2014; Wang

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et al., 2015; Yang et al., 2015; Pan et al., 2017) has been proposed to reduce the scale of SVM. In the SVM, the classifier is determined only by the so called "support vectors". The screening technique could identify most of the non-support vectors, and remove them before solving OPP. That saves the computational cost. One of the important advantages is that the solution obtained via screening method is exactly the same as the original problem. So this technique is regarded as a safe approach. In the literature (Wang et al., 2014), the method DVI (dual problem via variational inequalities) has shown its outstanding performance in the traditional SVM. However, the DVI rule cannot be simply applied to LapSVM. Specifically, the DVI-SVM only deals with one parameter C (Hastie et al., 2004), while there are multiple parameters in LapSVM.

Motivated by the studies above, in this paper a safe screening rule (SSR) is presented to accelerate LapSVM without sacrificing the optimal solution. At first, the Karush-Kuhn-Tucker (KKT) conditions are analyzed to motivate the proposed method. Then, via variational inequalities, the feasible set of the dual solution is constructed with the information obtained at the previous parameters. Combined the KKT conditions and the feasible set, the SSR is finally derived in an analytical form. By this rule, some components of the optimal solution could be achieved directly before solving QPP. Thus, the number of samples to be entered into the optimization problem can be substantially reduced. An important advantage of SSR-LapSVM is the safety, in the sense that the SSR is guaranteed to have the exactly same solution as solving the original LapSVM. In addition, by using Cholesky decomposition (Golub and Loan, 1996), the computational speed of inverse operation is improved. The effectiveness of our proposed method is verified by the experiments on both 3 artificial datasets and 24 real world benchmark datasets.

The main contributions of our method are summarized as follows:

- (i) By our screening rule, the scale of the optimization problem could be significantly reduced. Moreover, the solution is guaranteed to be exactly same as the original problem.
- (ii) Most existing screening rules only deal with one parameter problems. However, our screening rule can effectively address multiple parameter problems.
- (iii) Our screening rule is independent from the solvers, then some efficient methods can be embedded into it. In this paper, the dual coordinate descent method (DCDM) is chosen as the solving algorithm.

The rest of this paper is organized as follows: Section 2 gives related works. The SSR-LapSVM is proposed in Section 3. Experiments on artificial datasets and real world benchmark datasets are conducted to verify the excellence of our SSR-LapSVM in Section 4. The last section gives the conclusion.

# 2. Related works

For the supervised learning, consider a binary classification problem with a training set  $T = \{(x_1, y_1), (x_2, y_2), ..., (x_l, y_l)\}$ , where  $x_i \in \mathbb{R}^n$  is the input and  $y_i \in \{1, -1\}$  is the corresponding output. The traditional SVM searches for a separating hyper-plane  $f(x) = w^T \phi(x) + b = 0$ , where  $w \in \mathbb{R}^n$ ,  $b \in \mathbb{R}$ , and  $\phi(\cdot)$  is a nonlinear mapping to a higher dimensional Hilbert space. On one hand, maximizing the margin between two classes is equivalent to minimization of the regularization term  $\frac{1}{2} ||w||^2$ . On the other hand, training error  $L_{hinge}(x, y, f(x)) = max\{1 - yf(x), 0\}$  is minimized. Then, the following formulation is achieved:

$$\begin{split} \min_{w,b,\xi} &\quad \frac{1}{2} \|w\|^2 + C \sum_{i=1}^{i} \xi_i \\ \text{s.t.} &\quad y_i(w^T \phi(x_i) + b) \geq 1 - \xi_i, \\ &\quad \xi_i \geq 0, i = 1, 2, \dots, l, \end{split}$$

where C > 0 is a trade-off parameter.

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In SSL, a set of *l* labeled samples  $\{x_i, y_i\}_{i=1}^l$  and a set of *u* unlabeled samples  $\{x_i\}_{i=1+1}^{l+u}$  are given to train the model. LapSVM introduces an additional regularization term by using a graph Laplacian matrix L (Chova et al., 2008). The geometry of the data is modeled with a graph in which nodes represent both labeled and unlabeled samples connected by weights  $W_{ij}$  (Chapelle et al., 2006). Regularizing the graph follows from manifold assumption.

The decision function of LapSVM is given by  $f(x^*) = \langle w, \phi(x^*) \rangle + b =$  $\sum_{i=1}^{l+u} \alpha_i K(x_i, x^*) + b$ . K is the kernel matrix formed by kernel function  $K(x_i, x_j) = \langle \phi(x_i), \phi(x_j) \rangle$ . The regularization term can be expressed in terms of the kernel matrix and the expansion coefficients:  $||w||^2 = \alpha^T K \alpha$ . Finally, the formulation of LapSVM is written as:

$$\min_{\xi \in \mathbb{R}^{l}, \ \alpha \in \mathbb{R}^{l+u}} \quad \gamma_{1} \alpha^{T} K \alpha + \gamma_{2} \alpha^{T} K L K \alpha + e^{T} \xi$$
s.t. 
$$y_{i} K(x_{i}, x) \alpha \geq 1 - \xi_{i},$$

$$\xi_{i} \geq 0, \ i = 1, 2, \dots, l,$$
(1)

where  $\xi_i$  are slack variables to deal with errors in the labeled samples. Note that we let  $w = [w; b] \in \mathbb{R}^{n+1}$ ,  $x_i = [x_i, 1] \in \mathbb{R}^{n+1}$ .

Although the LapSVM has many admirable advantages, there is a difficulty to achieve the optimal parameters. The optimal values of  $\gamma_1$  and  $\gamma_2$  are unknown and it needs to estimate them. Commonly used model selection strategies such as cross validation and stability selection need to solve the optimization problems over a grid of turning parameters  $\{(\gamma_1^{(k)}, \gamma_2^{(k)})|, k = 1, 2, ..., T\}$  to determine appropriate values. This procedure is usually very time consuming.

To address this issue, in this paper a SSR is proposed for accelerating LapSVM. A block diagram for the whole scheme of the proposed method is given in Fig. 1. The repetitive process of parameter selection is denoted in red. The proposed screening process is denoted in green. Our goal is to safely reduce the optimization problem during the repetitive process of parameter selection.

#### 3. A safe screening rule for Laplacian support vector machine

In this section, the motivations for our method are given via KKT conditions. Then the feasible set is constructed via variational inequalities. The SSR is presented in the last subsection.

#### 3.1. Motivations

KKT conditions of LapSVM are studied to find out the instances which have no effect on the solution of the optimization problem.

The following Lagrangian function is introduced to solve QPP (1):

$$L(\alpha,\xi,\beta,\eta) = \gamma_1 \alpha^T K \alpha + \gamma_2 \alpha^T K L K \alpha + e^T \xi$$
  
- 
$$\sum_{i=1}^l \beta_i [y_i K(x_i,x)\alpha - 1 + \xi_i] - \sum_{i=1}^l \eta_i \xi_i,$$
 (2)

where  $\beta \ge 0$  and  $\eta \ge 0$  are the Lagrangian multipliers.

In the following,  $\alpha$ ,  $\beta$ ,  $\eta$  and  $\xi$  represent the feasible solutions.  $\alpha^*$ ,  $\beta^*$ ,  $\eta^*$  and  $\xi^*$  denote the corresponding optimal values.

Differentiating the Lagrangian function with respect to  $\alpha$  and  $\xi$  yields the following KKT conditions:

$$\frac{\partial L}{\partial \alpha} = 2\gamma_1 K \alpha^* + 2\gamma_2 K L K \alpha^* - \sum_{i=1}^l \beta_i^* y_i K(x_i, x) = \mathbf{0},\tag{3}$$

$$\frac{\partial L}{\partial \xi_i} = 1 - \beta_i^* - \eta_i^* = 0, \tag{4}$$

$$\beta_i^*(y_i K(x_i, x)\alpha^* - 1 + \xi_i^*) = 0, \tag{5}$$

$$q_i^* \xi_i^* = 0, \tag{6}$$

$$\beta_i^* \ge 0, \ \eta_i^* \ge 0, \ i = 1, 2, \dots, l.$$
 (7)



Fig. 1. The block diagram for the whole scheme of the proposed SSR-LapSVM. Our goal is to safely reduce the optimization problem in the process of parameter selection. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

From Eq. (3),  $\alpha^*$  can be represented as:

$$\alpha^* = (2\gamma_1 I + 2\gamma_2 L K)^{-1} J^T Y \beta^*, \tag{8}$$

where  $J = [I \ 0]$  is a  $l \times (l + u)$  matrix with I as the  $l \times l$  identity matrix and  $Y = \operatorname{diag}(y_1, \ldots, y_l)$ .

Let

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$$\mathcal{R} = \{i : y_i K(x_i, x) \alpha^* > 1\},\$$
  
$$\mathcal{E} = \{i : y_i K(x_i, x) \alpha^* = 1\},\$$
  
$$\mathcal{L} = \{i : y_i K(x_i, x) \alpha^* < 1\}.$$

From Eqs. (5), (6), (7) and the constraints of QPP (1), the following condition is obtained:

$$\beta_i^* = \begin{cases} 0, & \text{if } i \in \mathcal{R}; \\ [0, 1], & \text{if } i \in \mathcal{E}; \\ 1, & \text{if } i \in \mathcal{L}. \end{cases}$$
(9)

Substituting Eqs. (4) and (8) into (2), the following QPP is derived,

$$\min_{\boldsymbol{\beta} \in \mathbb{R}^{l}} \quad g(\boldsymbol{\beta}) = \frac{1}{2} \boldsymbol{\beta}^{T} \boldsymbol{Q} \boldsymbol{\beta} - \sum_{i=1}^{l} \boldsymbol{\beta}_{i}$$
s.t.  $0 \leq \boldsymbol{\beta}_{i} \leq 1, i = 1, 2, ..., l.$ 
(10)

where

$$Q = Y J K (2\gamma_1 I + 2\gamma_2 L K)^{-1} J^T Y.$$
 (11)

From (9), if some samples are known to be members of  $\mathcal{R}$  and  $\mathcal{L}$ , then the corresponding components of  $\beta^*$  can be set accordingly. So it only needs to determine the rest components of the variables. More precisely, the following Lemma 1 can be demonstrated easily.

**Lemma 1.** For the problem (10), given index sets  $\hat{\mathcal{R}} \subseteq \mathcal{R}$  and  $\hat{\mathcal{L}} \subseteq \mathcal{L}$ , we have

1.  $\beta_{\hat{\mathcal{R}}}^* = 0$  and  $\beta_{\hat{\mathcal{R}}}^* = 1$ . 2. Let  $\hat{S} = \hat{\mathcal{R}} \bigcup \hat{\mathcal{L}}, S = \mathcal{R} \bigcup \mathcal{L}, \hat{S}^C = S \setminus \hat{S}.$   $l' = |\hat{S}^C|$  denotes the cardinality of the set  $\hat{S}^{C}$ ,  $Q_{11} = Q_{\hat{S}^{C},\hat{S}^{C}}$ ,  $Q_{12} = Q_{\hat{S}^{C},\hat{S}}$  and  $\hat{f} = Q_{12}\beta_{\hat{S}} - e$ . e is the vector of ones of appropriate dimensions.

The reduced optimization problem is as follows,

$$\min_{\hat{\beta} \in \mathcal{R}^{\prime}} \quad \frac{1}{2} \hat{\beta}^T Q_{11}^T \hat{\beta} + \hat{f}^T \hat{\beta}$$

$$s.t. \quad 0 \le \hat{\beta} \le 1.$$
(12)

To implement LapSVM, it needs to solve the QPP (10). From Lemma 1, when  $\hat{S}$  is large, the computational cost for solving problem (12) can be much cheaper than solving the full problem (10). That motivates us to build the screening rule to reduce the computational cost.

#### 3.2. Feasible set construction

To reduce the computational cost, it needs to determine the membership of  $\hat{S}$ . The condition (9) seems to be useful. However, it is not applicable since  $\beta^*$  is unknown. To overcome this difficulty, a feasible region  $\Gamma$  such that  $\beta^* \in \Gamma$  is estimated. As a result, the relaxed version of (9) is derived,

$$\min_{\substack{\beta \in \Gamma}} y_i K(x_i, x) \alpha(\beta) > 1 \Rightarrow \beta_i^* = 0 \Leftrightarrow i \in \mathcal{R};$$

$$\max_{\substack{\beta \in \Gamma}} y_i K(x_i, x) \alpha(\beta) < 1 \Rightarrow \beta_i^* = 1 \Leftrightarrow i \in \mathcal{L};$$

$$(13)$$

where  $\alpha(\beta)$  changes with  $\beta$ . It can be obtained from (8).

Note that (13) serves as the foundation of the proposed SSR. In the subsequent sections, the feasible region  $\Gamma$  including  $\beta^*$  is estimated. Then the SSR is proposed based on this estimation and condition (13).

The main technique for estimating the region  $\Gamma$  is the so called variational inequalities. For self-completeness, the definition is cited as follows.

**Lemma 2** (*Güler*, 2010). Let  $A \subseteq \mathbb{R}^n$  be a convex set, and let g be a Gâteaux differentiable function on an open set containing A. If  $x^*$  is a local minimizer of g on A, then

$$\langle \nabla g(x^*), x - x^* \rangle \ge 0, \forall x \in A.$$

Via the variational inequalities, the following theorem shows that  $\beta^*(\gamma_1,\gamma_2)$  can be estimated in terms of  $\beta^*(\gamma_1^{(0)},\gamma_2^{(0)})$ . In the following,  $\beta^*(\gamma_1^{(0)}, \gamma_2^{(0)})$  and  $Q(\gamma_1^{(0)}\gamma_2^{(0)})$  are abbreviated as  $\beta^{*(0)}$  and  $Q^{(0)}$ , respectively.

**Theorem 3.** For problem (10), let  $\gamma_1 \ge \gamma_1^{(0)} > 0$ ,  $\gamma_2 \ge \gamma_2^{(0)} > 0$ . Assume  $GG^T = (2\gamma_1 K + 2\gamma_2 K L K)^{-1}$ ,  $G \in R^{(l+u) \times (l+u)}$  and  $Q = ZZ^T$  where  $Z = YJKG, Z \in R^{l \times (l+u)}$ . We have

$$\|Z^{T}\beta^{*} - \frac{Z^{-1}H}{2}\beta^{*(0)}\|^{2} \le \beta^{*(0)T}(\frac{1}{4}HQ^{-1}H - Q^{(0)})\beta^{*(0)},$$
(14)  
where  $H = Q^{(0)} + Q.$ 

Proof. The variational inequality implies that

$$\langle \nabla g(\beta^{*(0)}), \ \beta - \beta^{*(0)} \rangle \ge 0, \ \forall \beta \in [0,1]^l; \langle \nabla g(\beta^*), \ \beta - \beta^* \rangle \ge 0, \ \forall \beta \in [0,1]^l.$$

Notice that  $\beta^{*(0)}, \beta^* \in [0, 1]^l$ . It is easy to obtain the following result:

$$\langle \nabla g(\beta^{*(0)}), \ \beta^* - \beta^{*(0)} \rangle \ge 0; \langle \nabla g(\beta^*), \ \beta^{*(0)} - \beta^* \rangle \ge 0.$$
 (15)

From (15), the following result is obtained:

$$\langle \nabla g(\beta^{*(0)}) - \nabla g(\beta^{*}), \ \beta^{*} - \beta^{*(0)} \rangle \ge 0.$$
 (16)

Notice that  $\nabla g(\beta) = Q\beta - e$ . Plugging  $\nabla g(\beta^*)$  and  $\nabla g(\beta^{*(0)})$  into (16) leads to

$$\langle Q^{(0)}\beta^{*(0)} - Q\beta^{*}, \ \beta^{*} - \beta^{*(0)} \rangle \ge 0.$$

Then the following formulation is derived:

 $\beta^{*T} O^{(0)} \beta^{*(0)} - \beta^{*T} Q \beta^{*} - \beta^{*(0)T} Q^{(0)} \beta^{*(0)} + \beta^{*(0)T} Q \beta^{*} \ge 0.$ 

Assume  $GG^T = (2\gamma_1 K + 2\gamma_2 K L K)^{-1}$  and  $Q = ZZ^T$  where Z = YJKG, we can get

$$\|Z^{T}\beta^{*} - \frac{Z^{-1}(Q^{(0)} + Q)}{2}\beta^{*(0)}\|^{2} \leq \frac{1}{4}\beta^{*(0)T}(Q^{(0)} + Q)^{T}Q^{-1}(Q^{(0)} + Q)\beta^{*(0)} - \beta^{*(0)T}Q^{(0)}\beta^{*(0)}.$$
(17)

Let  $H = Q^{(0)} + Q$ , then (14) is demonstrated to be true.

# 3.3. A safe screening rule for LapSVM

Via Theorem 3, given  $\gamma_1 \ge \gamma_1^{(0)} > 0$  and  $\gamma_2 \ge \gamma_2^{(0)} > 0$ , the optimal solution  $\beta^*$  at  $(\gamma_1, \gamma_2)$  can be estimated in terms of the solution  $\beta^{*(0)}$  at  $(\gamma_1^{(0)}, \gamma_2^{(0)})$ . Based on this estimation, the basic screening rule for problem (10) is summarized in the following theorem:

**Theorem 4** (SSR). For problem (10), suppose we are given  $\beta^{*(0)}$ . Then, for any  $\gamma_1 > \gamma_1^{(0)} > 0$ ,  $\gamma_2 > \gamma_2^{(0)} > 0$ , we have  $\beta_i^* = 0$ , i.e.  $i \in \mathcal{R}$ , if the following holds

$$\frac{1}{2}H_{[i]}\beta^{*(0)} - Q_{ii}\sqrt{\beta^{*(0)T}(\frac{1}{4}HQ^{-1}H - Q^{(0)})\beta^{*(0)}} > 1.$$
  
Similarly, we have  $\beta_i^* = 1$ , i.e.  $i \in \mathcal{L}$ , if

$$\frac{1}{2}H_{[i]}\beta^{*(0)} + Q_{ii}\sqrt{\beta^{*(0)T}(\frac{1}{4}HQ^{-1}H - Q^{(0)})\beta^{*(0)}} < 1,$$

where  $H_{[i]}$  represents the *i*-th row of matrix H, and  $Q_{ii}$  is the *i*-th row *i*-th column element of matrix Q.

**Proof.** From (9) and Theorem 3, when  $y_i K(x_i, x) \alpha > 1$ , the following result can be derived:

$$\begin{split} y_i K(x_i, x) \alpha \\ &= y_i K(x_i, x) (2\gamma_1 I + 2\gamma_2 L K)^{-1} J^T Y \beta^* \\ &= y_i K(x_i, x) (2\gamma_1 K + 2\gamma_2 K L K)^{-1} K J^T Y \beta^* \\ &= y_i K(x_i, x) G G^T K J^T Y \beta^* \\ &= y_i K(x_i, x) G Z^T \beta^* \\ &= y_i K(x_i, x) G (Z^T \beta^* - \frac{1}{2} Z^{-1} H \beta^{*(0)}) + \frac{1}{2} y_i K(x_i, x) G Z^{-1} H \beta^{*(0)} \\ &\geq - \| y_i K(x_i, x) G \| \cdot \| Z^T \beta^* - \frac{1}{2} Z^{-1} H \beta^{*(0)} \| + \frac{1}{2} y_i K(x_i, x) G Z^{-1} H \beta^{*(0)} \\ &\geq - \| y_i K(x_i, x) G \| \cdot \sqrt{\beta^{*(0)T} (\frac{1}{4} H Q^{-1} H - Q^{(0)}) \beta^{*(0)}} \\ &+ \frac{1}{2} y_i K(x_i, x) G Z^{-1} H \beta^{*(0)} \\ &> 1. \end{split}$$

Note that, the second inequality is due to Theorem 3, and the last line is due to the statement. Finally, the inequality is obtained

$$\frac{1}{2}H_{[i]}\beta^{*(0)} - Q_{ii}\sqrt{\beta^{*(0)T}(\frac{1}{4}HQ^{-1}H - Q^{(0)})\beta^{*(0)}} > 1$$

When  $y_i K(x_i, x)\alpha < 1$ , the inequality (19) can be acquired similarly. This completes the proof.

The work flow of the proposed SSR is given in Fig. 2. At first, the primal and dual problems are analyzed by Karush–Kuhn–Tucker (KKT) conditions. Then, via variational inequalities, the feasible set of the dual solution is constructed with the information obtained at the previous parameters. Combined the KKT conditions and the feasible set, the SSR is finally derived in an analytical form. Through this rule, the scale of optimization problem at  $(\gamma_1, \gamma_2)$  is substantially reduced with the information obtained at  $(\gamma_1^{(0)}, \gamma_2^{(0)})$ .

In applications, it needs to estimate the optimal  $\gamma_1$  and  $\gamma_2$  and solve the optimization problem over a grid of turning parameters  $\{(\gamma_1^{(0)}, \gamma_2^{(0)}), (\gamma_1^{(1)}, \gamma_2^{(1)}), \dots, (\gamma_1^{(T)}, \gamma_2^{(T)})\}$  to determine appropriate values. Based on this procedure, a sequential version of the proposed SSR is presented below.

**Corollary 5** (Sequential SSR). For problem (10), suppose given a sequence of parameters  $\{(\gamma_1^{(k)}, \gamma_2^{(k)})|\gamma_1^{(k+1)} \ge \gamma_1^{(k)} > 0 \text{ and } \gamma_2^{(k+1)} \ge \gamma_2^{(k)} > 0, k = 0, \ldots, T-1\}$ . Assume  $\beta^{*(k)}$  is known for an arbitrary integer 1 < k < T. Then, for  $\beta^{*(k+1)}$ , we have  $\beta_i^{*(k+1)} = 0$ , i.e.  $i \in \mathcal{R}$ , if the following holds

$$-Q_{ii}^{(k+1)}\sqrt{\beta^{*(k)T}(\frac{1}{4}H^{(k+1)}(Q^{(k)})^{-1}H^{(k+1)} - Q^{(k)})\beta^{*(k)}} + \frac{1}{2}H_{[i]}^{(k+1)}\beta^{*(k)} > 1.$$
(18)

Similarly, we have  $\beta_i^{*(k+1)} = 1$ , i.e.  $i \in \mathcal{L}$ , if

$$\begin{aligned} \mathcal{Q}_{ii}^{(k+1)} \sqrt{\beta^{*(k)T} (\frac{1}{4} H^{(k+1)} (\mathcal{Q}^{(k)})^{-1} H^{(k+1)} - \mathcal{Q}^{(k)}) \beta^{*(k)}} \\ &+ \frac{1}{2} H_{[i]}^{(k+1)} \beta^{*(k)} < 1. \end{aligned}$$
(19)

The proposed SSR-LapSVM aims at accelerating original LapSVM. In our method, it needs to solve QPP (10) at  $(\gamma_1^{(0)}, \gamma_2^{(0)})$  and the reduced problems (12) at  $(\gamma_1^{(k)}, \gamma_2^{(k)})$ , k = 1, 2, ..., T. Since these problems are convex quadratic programming, their corresponding solutions are guaranteed to be globally optimal. The DCDM (Hsieh et al., 2008) is chosen to solve these optimization problems. Its convergence has been fully studied by Hsieh et al. (2008). It has been proved to reach an  $\epsilon$ accurate solution in  $O(\log(1/\epsilon))$  iterations. Meanwhile, via the proposed screening rule, the redundant instances in QPP (10) could be directly eliminated. Therefore, the effectiveness of the proposed methodology is guaranteed theoretically.

Note that  $(2\gamma_1 I + 2\gamma_2 LK)^{-1}$  in (8) and (11) can be written as  $(2\gamma_1 K + 2\gamma_2 KLK)^{-1}K^{-1}$ . Thus the ordinary matrix inverse operation is transformed to a symmetric matrix inverse operation. To further improve computational efficiency, it is computed by using Cholesky decomposition (Golub and Loan, 1996). To take care of the problem due to possible ill-condition, a term  $\epsilon I$  is added before the inverse operation, where  $\epsilon$  is a very small positive number and I is an identity matrix of appropriate dimensions.  $K^{-1}$  is calculated in initial step.

The pseudo code for SSR-LapSVM is presented in Algorithm 1, where  $P^{(k)}$  is a combination of  $(\gamma_1^{(k)}, \gamma_2^{(k)})$ . ID<sup>(k)</sup> denotes index of detected samples in each parameter selection step, and each element of  $\beta_{\text{ID}^{(k)}}^*$  is determined to be 0 or 1 before solving QPP (10).

Algorithm 1 SSR-LapSVM. **Input:**  $X_{\text{train}}, Y_{\text{train}}, X_{\text{test}}, Y_{\text{test}}, \gamma_1 \in \mathbb{R}^{r_1}, \gamma_2 \in \mathbb{R}^{r_2};$ **Output:**  $\gamma_1^*, \gamma_2^*$ , ID, Accuracy; **Initialization**: step = 0;  $ID^{(0)} = zeros(l, 1)$ ; calculate K,  $K^{-1}$ , L,  $P^{(k)}, k = 0, \dots, r_1 \times r_2 - 1;$ 1:  $\beta^{*(0)}, \alpha^{*(0)} \leftarrow \text{LapSVM with } P^{(0)};$ 2:  $f(x) \leftarrow \alpha^{*(0)};$ 3: Accuracy<sup>(0)</sup>  $\leftarrow$  predict( $f(x), X_{\text{test}}, Y_{\text{test}}$ ); Screening process: 4: **for** k = 0 to  $(r_1 \times r_2 - 1)$  **do**  $step \leftarrow step + 1;$ 5:  $ID^{(k+1)} \leftarrow put \beta^{*(k)}, P^{(k)}, P^{(k+1)} into (18) (19);$ 6:  $\hat{\beta}^{*(k+1)} \leftarrow \text{solve (12) with } P^{(k+1)}, \beta^{*}_{\text{ID}^{(k+1)}};$ 7:  $\beta^{*(k+1)} \leftarrow \text{combine } \hat{\beta}^{*(k+1)} \text{ and } \beta^{*}_{\mathrm{ID}^{(k+1)}};$ 8:  $\alpha^{*(k+1)} \leftarrow \text{put } \beta^{*(k+1)} \text{ into (8);}$ 9:  $f(x) \leftarrow \alpha^{*(k+1)};$ 10: Accuracy<sup>(k+1)</sup>  $\leftarrow$  predict( $f(x), X_{\text{test}}, Y_{\text{test}}$ ); 11: 12: end for γ<sub>1</sub><sup>\*</sup>, γ<sub>2</sub><sup>\*</sup> ← P<sup>\*</sup> corresponding to max(Accuracy);
 return γ<sub>1</sub><sup>\*</sup>, γ<sub>2</sub><sup>\*</sup>, ID, Accuracy

# 4. Numerical experiments

In this section, the numerical experiments are conducted on artificial datasets and real world datasets to demonstrate the validity of our proposed SSR-LapSVM. Artificial datasets are used to compare our proposed algorithm with traditional SVM and LapSVM. They include popular 2-circles dataset, 2-moons dataset<sup>1</sup> and a Gaussian distribution dataset. We further compare our proposed method with the state-of-the-art learning algorithms LapSVM, LapSVM-Newton, and LapSVM-PCG (Melacci and Belkin, 2011) on 24 benchmark datasets, such as USPS,<sup>2</sup> PCMAC,<sup>3</sup> Spambase,<sup>4</sup> Musk<sup>5</sup> and so on (Lichman, 2013; Chang and Lin, 2011). All of them are 2-class datasets except USPS. For USPS, some categories are taken out to be in 2-class version, including

<sup>&</sup>lt;sup>1</sup> http://www.dii.unisi.it/~melacci/lapsvmp/.

<sup>&</sup>lt;sup>2</sup> http://www.cs.nyu.edu/~roweis/data.html.

<sup>&</sup>lt;sup>3</sup> http://qwone.com/~jason/20Newsgroups/.

<sup>&</sup>lt;sup>4</sup> http://archive.ics.uci.edu/ml/datasets/Spambase.

<sup>&</sup>lt;sup>5</sup> http://archive.ics.uci.edu/ml/datasets/Musk + %28Version + 2%29.



**Fig. 2.** The work flow of the proposed SSR. The purpose is to determine the value of  $\beta^*$  with the information obtained at  $(\gamma_1^{(0)}, \gamma_2^{(0)})$ .



Fig. 3. Examples of 0, 3, 5, 6, 8 from USPS dataset.

USPS-3VS5, USPS-3VS8 and USPS-0VS6. Fig. 3 gives examples of USPS dataset.

All methods are implemented by using Matlab R2014a on Windows 7 running on a PC with system configuration Intel(R) Core(TM) 2 Duo CPU E7500 (2.93 GHz) with 8.00 GB of RAM. The package of LapSVM-Newton and LapSVM-PCG is downloaded from website.<sup>6</sup> The LapSVM and SSR-LapSVM are solved by DCDM.

The parameters related to build the graph Laplacian matrix (the number of neighbors and the degree) are fixed as specified by Melacci and Belkin (2011). The Laplacian matrix is computed using its normalized expression.

Gaussian kernel function  $k(x_i, x_j) = exp(-||x_i - x_j||^2/2\sigma^2)$  is considered as it is often applied and yields great generalization performance, where  $\sigma$  is a kernel parameter (Taylor and Cristianini, 2004; Cristianini and Shawe-Taylor, 2000). The parameter  $\sigma$  in SVM is selected over the range  $\{2^i | i = -5, -3..., 5\}$ . For the SSL methods, the kernel parameter is chosen according to the priori information (Melacci and Belkin, 2011).

#### 4.1. Artificial datasets

First, the popular two 2-D artificial datasets: 2-moons and 2-circles data are considered. There are only 2 labeled points for each class in two datasets. Parameters c,  $\gamma_1$  and  $\gamma_2$  in SVM, LapSVM and SSR-LapSVM are searched from set  $\{2^i | i = -5, -4, ..., 5\}$ . For the LapSVM and SSR-LapSVM, the kernel parameter  $\sigma$  is fixed as  $2^{-3}$  on 2-moons dataset and  $2^3$  on 2-circles dataset, respectively.

Illustrations of the algorithms with the optimal parameters are shown in Fig. 4. It can be observed that the supervised methods LapSVM and SSR-LapSVM have better prediction accuracy than the traditional SVM. More specifically, the SSR-LapSVM obtains the same solution as solving the LapSVM. Since the labeled samples are few, SSR-LapSVM works faster than LapSVM.

We further show that SSR-LapSVM is very effective in screening labeled samples even for largely overlapping classes. Our SSR-LapSVM is compared with the LapSVM on Gaussian distribution dataset, plotted in Fig. 5. We generate two classes of samples and each class has 500 labeled and 500 unlabeled data points. The dataset is generated from  $N(0.75, -0.75, 0.75^2, 0.75^2)$ . The blue dots represent positive class and the red dots represent the negative class.

Parameters  $\gamma_1$  and  $\gamma_2$  in LapSVM and SSR-LapSVM are searched from set  $\{2^i | i = -5, -4, \dots, 10\}$  and  $\{2^i | i = -5, -4, \dots, 5\}$ , respectively, and  $\sigma$ 

 Table 1

 The statistics of 24 benchmark datasets.

Dataset	#Sample	#Feature	#Training	#Testing		
Dataset	bampic	reature	Labeled	Unlabeled	resting	
DBWorld	64	4702	26	15	13	
Fertility	100	9	40	40	20	
LSVT	126	310	51	50	25	
PlanningRelax	146	12	73	73	36	
Sonar	208	60	84	84	40	
SpectHeart	267	44	107	107	53	
BCIa	268	5376	107	107	54	
Haberman	306	4	123	122	61	
LiverDisorder	345	6	138	138	69	
Ionosphere	351	34	141	140	70	
Monks	432	6	173	172	87	
BreastCancer569	569	30	227	227	115	
BreastCancer683	683	274	273	9	136	
Australian	690	14	276	275	139	
Pima	768	8	308	307	153	
Banknote	1372	4	549	548	275	
USPS-3VS8	1532	256	50	1175	307	
USPS-3VS5	1540	256	50	1182	308	
PCMAC	1943	3289	200	1354	389	
USPS-0VS6	2387	256	50	1859	478	
Adult	3185	122	1274	1274	637	
Spambase	4601	57	500	3182	919	
Musk	6598	166	2640	2639	1319	
Mushroom	8124	112	3250	3249	1625	

is fixed as 0.125. The optimal classifier of LapSVM is presented on the Toy dataset in Fig. 5(a). Figs. 5(b), 5(c) and 5(d) are illustrations of SSR-LapSVM in different parameter selection steps. Green points represent the detected points in advance of solving QPP. The total computational time of SSR-LapSVM is 257.0591 s. By contrast, the running time of original LapSVM is 371.1248 s which is slower over 114 s than our methods.

Fig. 6(a) indicates that our SSR-LapSVM always has the same accuracy as LapSVM in each step, which also demonstrates that the process of data screening is guaranteed to have the exactly same solution as the original LapSVM.

Fig. 6(b) gives detailed ratio of detected labeled points along with the selecting parameter steps. With the increase of steps, there is a growing number of detected labeled points. Fig. 6(b) indicates that the proposed methods can identify almost all of the labeled points.

#### 4.2. Benchmark datasets

In this experiment, we compare our SSR-LapSVM with semisupervised algorithms LapSVM, LapSVM-Newton and LapSVM-PCG in terms of prediction accuracy and computational time. These algorithms are implemented along a sequence of 40 × 40 parameter combinations of  $\gamma_1, \gamma_2 \in [2^{-5}, 2^{10}]$  equally spaced in the logarithmic scale.

The statistics of benchmark datasets are given in Table 1. Each dataset is divided into two parts: training data and testing data. The training set is composed of labeled and unlabeled data. In our experiments, 4/5 of positive samples and 4/5 of negative samples are randomly selected as the training set, in which the labels of the training data are randomly deleted with a certain proportion. The rest samples are reserved as a testing set.

<sup>&</sup>lt;sup>6</sup> http://www.dii.unisi.it/~melacci/lapsvmp/.



Fig. 4. Performance comparisons of SVM, LapSVM, and SSR-LapSVM on 2-moons and 2-circles datasets.



Fig. 5. Classification maps of LapSVM and SSR-LapSVM on Toy dataset. (a) LapSVM with the optimal parameters, (b) SSR-LapSVM in parameter selection step 2, (c) SSR-LapSVM in parameter selection step 9, (d) SSR-LapSVM in parameter selection step 10. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)



Fig. 6. Results of LapSVM and SSR-LapSVM on Toy dataset.

Take the last dataset "Mushroom" as an example. This dataset includes 8124 samples corresponding to 23 species of gilled mushrooms in the Agaricus and Lepiota Family (Lichman, 2013). Each species is identified as edible (3916 positive samples) or poisonous (4208 negative samples). In our experiment, 3133 positive data (4/5 of 3916) and 3366 negative data (4/5 of 4208) are randomly collected as the training set (in total 6499 samples) and the rest samples are reserved as testing set. To make the unlabeled ratio as 50%, the labels of 3250 (50% of 6499) training data are randomly deleted.

Table 2 gives the detailed comparisons of our SSR-LapSVM and LapSVM on 24 benchmark datasets. Where "Average" denotes average time of each parameter selection step; "Initialization" represents the initialization time which is the cost for constructing matrixes; "Inverse" denotes average time of matrix inverse operation in each step; "Solver" represents the average time of solving QPP in each parameter selection step of LapSVM, and in SSR-LapSVM it contains the time of both screening process and solving QPP; "SSR Ratio(%)" is only for SSR-LapSVM, which represents the average ratio of detected samples in each

## Table 2

Detailed	comparisons	of SSR-La	nSVM and	LanSVM on 2	4 henchmark	datasets	Bold type shows the best result
Julancu	companisons	or obit-La	po v ivi and	Lapo vivi on 2	27 Deneminark	uatasets.	Dola type shows the best result.

		Time(s)						
Dataset	Algorithm	Average Initialization		Inverse	Solver	SSR Ratio(%)	Speedup	
	LanSVM	0.0225	0.0013	0.0204	0.0006			
DBWorld	SSR-LapSVM	0.0019	0.0001	0.0013	0.0003	79.08	11.84	
	LapSVM	0.0533	0.0016	0.0192	0.0231			
Fertility	SSR-LapSVM	0.0033	0.0004	0.0011	0.0012	63.02	16.15	
	LapSVM	0.0012	0.0002	0.0004	0.0004			
LSVT	SSR-LapSVM	0.0047	0.0003	0.0019	0.0018	65.34	0.26	
	LapSVM	0.2722	0.0047	0.1195	0.1082			
PlanningRelax	SSR-LapSVM	0.0057	0.0013	0.0013	0.0027	68.02	47.75	
	LapSVM	0.0063	0.0013	0.0023	0.0023			
Sonar	SSR-LapSVM	0.0025	0.0004	0.0009	0.0008	70.70	2.52	
0	LapSVM	0.2727	0.0021	0.0763	0.1784		07.00	
SpectHeart	SSR-LapSVM	0.0072	0.0017	0.0026	0.0024	68.27	37.88	
DO	LapSVM	0.5988	0.0045	0.1870	0.3672		50.1.4	
BCIa	SSR-LapSVM	0.0083	0.0015	0.0034	0.0029	72.91	72.14	
** 1	LapSVM	1.5035	0.0063	0.2068	1.2576		60 0 <b>7</b>	
Haberman	SSR-LapSVM	0.0218	0.0022	0.0044	0.0145	54.54	68.97	
·· · · ·	LapSVM	0.0139	0.0037	0.0055	0.0038		1.01	
LiverDisorder	SSR-LapSVM	0.0077	0.0009	0.0034	0.0006	73.92	1.81	
T	LapSVM	0.4721	0.0049	0.1481	0.2966		45.00	
Ionosphere	SSR-LapSVM	0.0104	0.0019	0.0041	0.0040	65.13	45.39	
Maula	LapSVM	0.0244	0.0064	0.0092	0.0076		0.54	
MORKS	SSR-LapSVM	0.0096	0.0011	0.0026	0.0030	62.88	2.54	
B	LapSVM	0.6752	0.0122	0.2506	0.3811		05 54	
BreastCancer569	SSR-LapSVM	0.0190	0.0036	0.0071	0.0069	58.62	35.54	
D	LapSVM	0.5109	0.0113	0.2120	0.2637		10.00	
BreastCancer683	SSR-LapSVM	0.0258	0.0048	0.0100	0.0092	53.07	19.80	
A	LapSVM	0.8132	0.0173	0.3936	0.3678		01.64	
Australian	SSR-LapSVM	0.0257	0.0047	0.0098	0.0093	65.77	31.64	
Dime	LapSVM	0.8269	0.0156	0.3984	0.3789		07.04	
Australian Pima	SSR-LapSVM	0.0296	0.0049	0.0121	0.0104	52.00	27.94	
Dealasta	LapSVM	0.1720	0.0196	0.0579	0.0824		0.05	
Banknote	SSR-LapSVM	0.2014	0.0056	0.1129	0.0126	44.93	0.85	
LICDC OVCO	LapSVM	0.3511	0.0297	0.2511	0.0503		4 70	
0525-3758	SSR-LapSVM	0.0742	0.0094	0.0611	0.0029	78.09	4.73	
LICDC OVCE	LapSVM	0.3168	0.0300	0.2214	0.0463		1	
USPS-3VS5	SSR-LapSVM	0.0575	0.0096	0.0441	0.0030	78.18	5.51	
DOMAG	LapSVM	1.2427	0.1313	0.8970	0.1803		0.01	
PCMAC	SSR-LapSVM	0.4423	0.0838	0.3055	0.0492	69.00	2.81	
LICDC OVEC	LapSVM	0.9014	0.0713	0.7281	0.0722		2.22	
03P3-0V30	SSR-LapSVM	0.2796	0.0178	0.2559	0.0044	77.75	3.22	
4 1.14	LapSVM	3.5515	0.4356	0.5056	2.5181		1 10	
Adult	SSR-LapSVM	2.9751	0.1745	0.5054	1.7946	34.83	1.19	
0	LapSVM	1.9868	0.0511	0.9296	0.9664		1.00	
spainbase	SSR-LapSVM	1.0155	0.0557	0.8788	0.0554	66.61	1.90	
Much	LapSVM	17.6137	0.3324	3.5774	13.1059		1.07	
WIUSK	SSR-LapSVM	16.5305	0.1081	3.0824	12.7604	20.04	1.07	
Mushaoon	LapSVM	20.3176	0.3588	6.5672	12.3418		2.26	
Mushroom	SSR-LapSVM	8.5976	0.0119	5.5649	2.0454	42.21	2.30	

# step. "Speedup" denotes

Speedup -	Time of SSR-LapSVM	
speedup =	The second second	•

```
Time of LapSVM
```

From the columns of "Average" and "Speedup" in Table 2, the average speed of each step of SSR-LapSVM is many times faster than that of LapSVM. From the column of "Solver", we observe that the solver of proposed SSR-LapSVM is obviously faster than LapSVM. It indicates that SSR truly contributes to improving the speed of solving QPP. From the column of "Inverse", we find that our SSR-LapSVM runs faster than LapSVM in the inverse operation. It indicates that the fast inverse operation technique indeed works efficiently. From the column of "SSR Ratio", we see that SSR-LapSVM can generally detect most of the label samples before solving QPP. By contrast, the original LapSVM does not have this function.

Table 3 shows the performance comparisons of four algorithms on 24 benchmark datasets. Where "Accuracy(%)" represents the prediction accuracy with the optimal values of parameters, and "Time(s)" denotes its corresponding time.

From Table 3, we find that the accuracy of our SSR-LapSVM is almost the same as original LapSVM on each dataset. It demonstrates that SSR-LapSVM is truly a safe algorithm to guarantee the same solution as solving the original LapSVM. By contrast, LapSVM-Newton and LapSVM-PCG do not have this property. In terms of running time, SSR-LapSVM and LapSVM-PGC are generally faster than LapSVM-Newton and LapSVM.

In general, our proposed SSR-LapSVM could greatly accelerate the LapSVM. Moreover, it guarantees to obtain the same predication accuracy as the original LapSVM.

# 5. Conclusion

In this paper, an efficient SSR for LapSVM is proposed via variational inequalities. It can greatly reduce the number of training samples and effectively improve the computational speed. Moreover the same solution can be achieved as solving the original problem, so it is safe. In comparison with the existing DVI-SVM, it effectively addresses the problem of multiple parameters. Experiments on both 3 artificial datasets and 24 real world benchmark datasets demonstrate its feasibility and validity. The SSR only screens the labeled samples, how to screen the unlabeled instances is our further work.

Table 3

Performance comparisons of four algorithms on 24 benchmark datasets. Bold type shows the best result.

Dataset	LapSVM-Newton		LapSVM-PCG		LapSVM		SSR-LapSVM	
	Accuracy(%)	Time(s)	Accuracy(%)	Time(s)	Accuracy(%)	Time(s)	Accuracy(%)	Time(s)
DBWorld	61.54	0.0044	61.54	0.0026	61.54	0.0073	61.54	0.0022
Fertility	90.00	0.0043	90.00	0.0029	95.00	0.0204	95.00	0.0020
LSVT	88.00	0.0041	88.00	0.0034	88.00	0.0013	88.00	0.0065
PlanningRelax	72.22	0.0058	72.22	0.0032	72.22	0.0231	72.22	0.0101
Sonar	70.00	0.0062	75.00	0.0042	100.00	0.0089	100.00	0.0059
SpectHeart	86.79	0.0074	86.79	0.0061	86.79	0.0408	86.79	0.0073
BCIa	72.22	0.0550	72.22	0.0106	77.78	0.8034	77.78	0.0081
Haberman	80.33	0.0089	80.33	0.0074	80.33	2.7046	80.33	0.0227
LiverDisorder	71.01	0.0041	71.01	0.0077	71.01	0.0204	71.01	0.0063
Ionosphere	88.57	0.0117	88.57	0.0071	90.00	0.0101	90.00	0.0110
Monks	89.66	0.0058	89.66	0.0224	82.76	0.0223	82.76	0.0096
BreastCancer569	94.78	0.2065	93.91	0.0206	98.26	0.5041	98.26	0.0861
BreastCancer683	97.79	0.2249	98.53	0.0266	98.53	0.2070	98.53	0.0234
Australian	64.03	0.1516	64.03	0.0225	87.77	0.0900	87.77	0.0311
Pima	75.82	0.0383	73.86	0.0358	76.47	0.0409	76.47	0.0362
Banknote	100.00	0.1637	100.00	0.2107	100.00	0.1920	100.00	0.1974
USPS-3VS8	99.02	0.2420	99.02	0.2467	100.00	0.1127	100.00	0.0797
USPS-3VS5	95.45	0.2388	95.45	0.2513	100.00	0.2227	100.00	0.0536
PCMAC	83.03	0.7980	83.03	0.8469	89.46	0.4310	89.46	0.3963
USPS-0VS6	99.73	0.5235	99.70	0.5771	100.00	0.4131	100.00	0.2206
Adult	84.93	2.3286	84.93	2.1533	84.30	3.4354	84.30	2.1750
Spambase	78.56	2.6920	78.56	2.6847	92.06	1.8951	92.06	1.0294
Musk	95.60	6.1524	95.60	6.1611	98.64	35.8633	98.64	31.9621
Mushroom	100.00	86.1518	100.00	179.4507	100.00	21.6847	100.00	7.8820

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