

ARTICLE TITLE

JOHN SMITH* & JAMES SMITH¹

CONTENTS

1	Introduction	2
1.1	Margin	2
2	SVM: non-separable case	2
2.1	Formulation I	2
2.2	Formulation II	3
2.3	With Kernel	4
3	Lasso	4
3.1	Formulation I	4
3.2	Formulation II	5
4	Methods	5
5	REAPER	5
5.1	Parameters of REAPER	6
6	Results and Discussion	6

LIST OF FIGURES

LIST OF TABLES

ABSTRACT

* *Department of Biology, University of Examples, London, United Kingdom*

¹ *Department of Chemistry, University of Examples, London, United Kingdom*

1 INTRODUCTION

My current plan is to write a survey about the screening methods used in identifying non-support vector in solving Support Vector Machine (SVM) problem. Such methods differ from the screening strategy for lasso in that, in SVM the data points are discarded while in lasso the features are discarded.

1.1 Margin

Given a hyperplane $\mathcal{H} = \{\mathbf{x} \in \mathbb{R}^d : \mathbf{w} \cdot \mathbf{x} + b = 0\}$, the distance from a point $\mathbf{z} \in \mathbb{R}^d$ to \mathcal{H} is $\mathbf{D}(\mathbf{z}, \mathcal{H}) = \frac{\mathbf{w} \cdot \mathbf{z} + b}{\|\mathbf{w}\|}$. If we know whether the point is above or below the hyperplane by the sign variable $y \in \{-1, +1\}$, we define the margin to be $\mathbf{M}(\mathbf{z}, \mathcal{H}) = y \frac{\mathbf{w} \cdot \mathbf{z} + b}{\|\mathbf{w}\|}$.

Now suppose we are given a dataset $\mathcal{X} = \{y_i, \mathbf{x}_i\}_{i=1}^m$, the margin of \mathcal{X} to \mathcal{H} is defined as

$$\mathbf{M}(\mathcal{X}, \mathcal{H}) = \min_{\mathbf{z} \in \mathcal{X}} \mathbf{M}(\mathbf{z}, \mathcal{H}).$$

Given that the dataset \mathcal{X} is separable, SVM aims to seek a hyperplane \mathcal{H}^* that gives the largest margin of \mathcal{X} to \mathcal{H}^* . Such goal can be formalized as

$$\begin{aligned} \max_{\mathcal{H}} \quad & \rho \\ \text{s.t.} \quad & \mathbf{M}(\mathbf{z}, \mathcal{H}) \geq \rho, \forall \mathbf{z} \in \mathcal{X} \end{aligned}$$

Clearly we can scale \mathbf{w} and b such that $\min_{\mathbf{z} \in \mathcal{X}} |\mathbf{z} \cdot \mathbf{w} + b| = 1$, thus the above formulation is equivalent to

$$\begin{aligned} \min \quad & \|\mathbf{w}\| \\ \text{s.t.} \quad & y_i(\mathbf{x}_i \cdot \mathbf{w} + b) \geq 1, i = 1, \dots, m \end{aligned} \tag{1}$$

2 SVM: NON-SEPARABLE CASE

We are interested in solving SVM problem where there is no hyperplane that can correctly classify all the data points. There are several formulations of SVM whose primal and dual problems, KKT conditions, and corresponding screening properties will be discussed one by one.

2.1 Formulation I

The primal formulation of such problem is

$$\begin{aligned} \min_{\mathbf{w}, b, \xi} \quad & \frac{1}{2} \|\mathbf{w}\|_2^2 + C \sum_{i=1}^m \xi_i^\beta \\ \text{s.t.} \quad & y_i(\mathbf{w} \cdot \mathbf{x}_i + b) \geq 1 - \xi_i, \xi_i \geq 0, i \in [m]. \end{aligned} \tag{P}_\beta^I$$

where $\beta = 1$ or 2 , corresponding to l_1 and l_2 SVM variants.

It is clear that when $\beta = 1$, the l_1 -SVM problem is equivalent to the following problem.

$$\min_{\mathbf{w}, b} \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1}^m [1 - y_i(\mathbf{w} \cdot \mathbf{x}_i + b)]_+ \tag{2}$$

Using the standard derivation, we have the following dual formulation of (P_β^I) when $\beta = 1$

$$\begin{aligned} \max_{\alpha} \quad & \|\alpha\|_1 - \frac{1}{2} \alpha^\top Q \alpha \\ \text{s.t.} \quad & 0 \leq \alpha_i \leq C, \alpha \cdot y = 0, i \in [m], \end{aligned} \quad (D_1^I)$$

where $Q_{i,j} = y_i y_j (x_i \cdot x_j)$. Given a primal solution w^*, ξ^*, b^* and a dual solution α^* , the KKT condition states that

1. $\xi_i^* \geq 0, i = 1, \dots, m$.
2. $\xi_i^* \geq 1 - y_i(w^* \cdot x_i + b^*), i = 1, \dots, m$
3. $0 \leq \alpha_i^* \leq C, i = 1, \dots, m$
4. $\alpha_i^*(1 - y_i(w^* \cdot x_i + b^*) - \xi_i^*) = 0, i = 1, \dots, m$
5. $(C - \alpha_i^*)\xi_i^* = 0, i = 1, \dots, m$
6. $w^* = A\alpha^*$

where $A = [\dots y_i x_i \dots]_i$.

If $1 - y_i(w^* \cdot x_i + b^*) < 0$ then $(1 - y_i(w^* \cdot x_i + b^*) - \xi_i^*) < 0$, we have $\alpha_i^* = 0$ by the complementary slackness. Similarly, if $1 - y_i(w^* \cdot x_i + b^*) > 0$, we have $\alpha_i^* = C$. By categorizing the m training instances into three sets

- $\mathcal{R} := \{i \in [m] | y_i(w^* \cdot x_i + b) > 1\}$
- $\mathcal{E} := \{i \in [m] | y_i(w^* \cdot x_i + b) = 1\}$
- $\mathcal{L} := \{i \in [m] | y_i(w^* \cdot x_i + b) < 1\}$

we summarize such property by that

- $i \in \mathcal{R} \rightarrow \alpha_i = 0$
- $i \in \mathcal{E} \rightarrow \alpha_i \in [0, C]$
- $i \in \mathcal{L} \rightarrow \alpha_i = C$

2.2 Formulation II

Another way to write SVM is by

$$\begin{aligned} \min_{w, b, \xi} \quad & \frac{1}{2} \|w\|_2^2 \\ \text{s.t.} \quad & y_i(w \cdot x_i + b) \geq 1 - \xi_i, \xi_i \geq 0, i \in [m] \\ & \sum_{i=1}^m \xi_i \leq s, \end{aligned} \quad (P_\beta^{II})$$

which is clearly equivalent to the following problem when we take $\beta = 1$

$$\begin{aligned} \min_{w, b} \quad & \frac{1}{2} \|w\|^2 \\ \text{s.t.} \quad & \sum_{i=1}^m [1 - y_i(w \cdot x_i + b)]_+ \leq s. \end{aligned} \quad (3)$$

where $[a]_+ = \max\{a, 0\}$ denotes the hinge loss.

Using the standard derivation, we have the following dual formulation of (P_β^{II}) when $\beta = 1$

$$\begin{aligned} \max_{\alpha, C} \quad & \|\alpha\|_1 - \frac{1}{2} \alpha^\top Q \alpha - Cs \\ \text{s.t.} \quad & 0 \leq \alpha_i \leq C \cap \alpha \cdot y = 0, i \in [m], \end{aligned} \quad (D_1^{II})$$

Given a primal solution w^*, ξ^*, b^* and a dual solution α^*, C^* , the KKT condition states that

1. $\xi_i^* \geq 0, i = 1, \dots, m.$
2. $\xi_i^* \geq 1 - y_i(w^* \cdot x_i + b^*), i = 1, \dots, m$
3. $\sum_{i=1}^m \xi_i^* \leq s$
4. $0 \leq \alpha_i^* \leq C^*, i = 1, \dots, m$
5. $C^* \geq 0$
6. $(\sum_{i=1}^m \xi_i^* - s)C^* = 0$
7. $\alpha_i^*(1 - y_i(w^* \cdot x_i + b^*) - \xi_i^*) = 0, i = 1, \dots, m$
8. $(C^* - \alpha_i^*)\xi_i^* = 0, i = 1, \dots, m$
9. $w^* = A\alpha^*$

where $A = [\dots y_i x_i \dots]_i$.

I have not yet figure out the screening properties in this formulation.

2.3 With Kernel

3 LASSO

3.1 Formulation I

Primal:

$$\begin{aligned} \min_x \quad & \frac{1}{2} \|Ax - b\|^2 \\ \text{s.t.} \quad & \|x\|_1 \leq t \end{aligned} \quad (4)$$

which is equivalent to

$$\begin{aligned} \min_x \quad & \frac{1}{2} \|z\|^2 \\ \text{s.t.} \quad & \|x\|_1 \leq t \cap Ax - b = z \end{aligned} \quad (5)$$

Dual of 5:

$$\begin{aligned} \max_{\theta, \lambda} \quad & \frac{\|b\|^2}{2} - \frac{\|\theta - b\|^2}{2} - \lambda t \\ \text{s.t.} \quad & \|A^\top \theta\|_\infty \leq \lambda \end{aligned} \quad (6)$$

Given a primal solution x^*, z^* and dual solution θ^*, λ^* KKT condition states:

- $\|x^*\|_1 \leq t \cap Ax^* - b^* = z^*$
- $\lambda \geq 0$

- $\mathbf{z}^* + \boldsymbol{\theta}^* = 0$
- $\frac{\mathbf{A}^\top \boldsymbol{\theta}^*}{\lambda^*} \in \partial \|\mathbf{x}^*\|_1$
- $\lambda(\|\mathbf{x}^*\|_1 - t) = 0$

From the fourth property, we have that if $|\mathbf{A}_i \cdot \boldsymbol{\theta}^*| < \lambda^*, \mathbf{x}_i^* = 0$.

3.2 Formulation II

Primal:

$$\min_{\mathbf{x}} \quad \frac{1}{2} \|\mathbf{Ax} - \mathbf{b}\|^2 + \lambda \|\mathbf{x}\|_1 \quad (7)$$

which is equivalent to

$$\begin{aligned} \min_{\mathbf{x}} \quad & \frac{1}{2} \|\mathbf{z}\|^2 + \lambda \|\mathbf{x}\|_1 \\ \text{s.t.} \quad & \mathbf{Ax} - \mathbf{b} = \mathbf{z} \end{aligned} \quad (8)$$

Dual of 8:

$$\begin{aligned} \max_{\boldsymbol{\theta}} \quad & \frac{\|\mathbf{b}\|^2}{2} - \frac{\|\boldsymbol{\theta} - \mathbf{b}\|^2}{2} \\ \text{s.t.} \quad & \|\mathbf{A}^\top \boldsymbol{\theta}\|_\infty \leq \lambda \end{aligned} \quad (9)$$

Given a primal solution $\mathbf{x}^*, \mathbf{z}^*$ and dual solution $\boldsymbol{\theta}^*$ KKT condition states:

- $\mathbf{Ax}^* - \mathbf{b}^* = \mathbf{z}^*$
- $\frac{\mathbf{A}^\top \boldsymbol{\theta}^*}{\lambda} \in \partial \|\mathbf{x}^*\|_1$

From the fourth property, we have that if $|\mathbf{A}_i \cdot \boldsymbol{\theta}^*| < \lambda, \mathbf{x}_i^* = 0$.

4 METHODS

Support function for a ball $\mathbf{B}(\mathbf{c}, r) = \{\mathbf{x} \mid \|\mathbf{x} - \mathbf{c}\| \leq r\}$

$$\mathbf{H}_{\mathbf{B}(\mathbf{c}, r)}(\mathbf{a}) = \sup_{\mathbf{x} \in \mathbf{B}(\mathbf{c}, r)} \mathbf{a} \cdot \mathbf{x} = \mathbf{a} \cdot \mathbf{c} + r \quad (10)$$

5 REAPER

Principal Component Analysis can be formalized as

$$\begin{aligned} \min_{\Pi} \quad & \sum_{\mathbf{x} \in \mathcal{X}} \|\mathbf{x} - \Pi \mathbf{x}\|^2 \\ \text{s.t.} \quad & \Pi \text{ is an orthoprojector} \cap \text{tr} \Pi = d \end{aligned} \quad (11)$$

which can be readily solved by Singular Value Decomposition (SVD) in a closed form. However, such formulation is not robust to outliers. One alternative is to replace square residual with residual, that is

$$\begin{aligned} \min_{\Pi} \quad & \sum_{\mathbf{x} \in \mathcal{X}} \|\mathbf{x} - \Pi \mathbf{x}\| \\ \text{s.t.} \quad & \Pi \text{ is an orthoprojector} \cap \text{tr} \Pi = d \end{aligned} \quad (12)$$

Unfortunately, the constrain is non-convex which makes the problem difficult to solve.

Convex Relaxation is often utilized so that efficient solvers can be used. In REAPER, the constrain is relaxed to its convex hull, i.e.

$$\begin{aligned} \min_{\mathbf{P}} \quad & \sum_{\mathbf{x} \in \mathcal{X}} \|\mathbf{x} - \mathbf{P}\mathbf{x}\| \\ \text{s.t.} \quad & 0 \preceq \mathbf{P} \preceq \mathbf{I} \cap \text{tr} \mathbf{P} = d \end{aligned} \quad (13)$$

Clearly, the solution \mathbf{P}^* to 13 may not be feasible in the original problem 12, REAPER outputs the solution to the following problem

$$\begin{aligned} \min_{\Pi} \quad & \|\mathbf{P}^* - \Pi\|_{S_1} \\ \text{s.t.} \quad & \Pi \text{ is an orthoprojector} \cap \text{tr} \Pi = d \end{aligned} \quad (14)$$

5.1 Parameters of REAPER

Let $\mathbf{M} \subset \mathbb{R}^D$ be a subspace, let Π and Π^\perp be the corresponding orthoprojectors to \mathbf{M} and \mathbf{M}^\perp . Define the following parameters.

Permeance Statistic $\mathcal{P}(\mathbf{M})$:

$$\mathcal{P}(\mathbf{M}) := \inf_{\mathbf{u} \in \mathbf{M}, \|\mathbf{u}\|=1} \sum_{\mathbf{x} \in \mathcal{X}_{\text{in}}} |\langle \mathbf{u}, \Pi \mathbf{x} \rangle| \quad (15)$$

Total Inlier Residual $\mathcal{R}(\mathbf{M})$:

$$\mathcal{R}(\mathbf{M}) := \sum_{\mathbf{x} \in \mathcal{X}_{\text{in}}} \|\Pi^\perp \mathbf{x}\|. \quad (16)$$

Alignment Statistic $\mathcal{A}(\mathbf{M})$:

$$\mathcal{A}(\mathbf{M}) := \|\mathbf{X}_{\text{out}}\| \cdot \|\mathcal{S}(\Pi^\perp \mathbf{X}_{\text{out}})\|. \quad (17)$$

where $\mathcal{S}(\mathbf{A})$ spherizes the columns of the matrix \mathbf{A} . and the *Stability Statistic* $\Phi(\mathbf{M})$:

$$\Phi(\mathbf{M}) := \frac{\mathcal{P}(\mathbf{M})}{4\sqrt{\dim(\mathbf{M})}} - \mathcal{A}(\mathbf{M}). \quad (18)$$

6 RESULTS AND DISCUSSION

REFERENCES