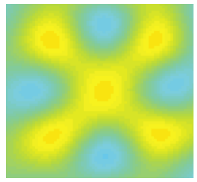

BSVM

A Banded Support Vector Machine

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Contents

List of Figures

Abstract

We describe a novel binary classification technique called Banded SVM (B-SVM). In the standard C-SVM formulation of Cortes and Vapnik [1995], the decision rule is encouraged to lie in the interval $[1, \infty]$. The new B-SVM objective function contains a penalty term that encourages the decision rule to lie in a user specified range $[\rho_1, \rho_2]$. In addition to the standard set of support vectors (SVs) near the class boundaries, B-SVM results in a second set of SVs in the interior of each class.

Notation

- Scalars and functions will be denoted in a non-bold font (e.g., β_0, C, g). Vectors and vector functions will be denoted in a bold font using lower case letters (e.g., $\boldsymbol{x}, \boldsymbol{\beta}, \boldsymbol{h}$). Matrices will be denoted in bold font using upper case letters (e.g., $\boldsymbol{B}, \boldsymbol{H}$). The transpose of a matrix $\boldsymbol{A}$ will be denoted by $\boldsymbol{A^T}$ and its inverse will be denoted by $\boldsymbol{A^{-1}}$. $\boldsymbol{I_p}$ will denote the $p \times p$ identity matrix and $\mathbf{0}$ will denote a vector or matrix of all zeros whose size should be clear from context.

- $|x|$ will denote the absolute value of x and $\mathcal{I}(x > a)$ is an indicator function that returns 1 if $x > a$ and 0 otherwise.

- The jth component of vector $\boldsymbol{t}$ will be denoted by t_j. The element (i, j) of matrix $\boldsymbol{G}$ will be denoted by $G(i, j)$ or G_{ij}. The 2-norm of a $p \times 1$ vector $\boldsymbol{x}$ will be denoted by $||\boldsymbol{x}||_2 = +\sqrt{\sum_{i=1}^{p} x_i^2}$. Probability distribution of a random vector $\boldsymbol{x}$ will be denoted by $\mathbf{P}_{\boldsymbol{x}}(\boldsymbol{x})$. $\mathbf{E}[f(\boldsymbol{s}, \boldsymbol{\eta})]$ denotes the expectation of $f(\boldsymbol{s}, \boldsymbol{\eta})$ with respect to both random variables $\boldsymbol{s}$ and $\boldsymbol{\eta}$.

1 Introduction

We consider the standard binary classification problem. Suppose y_i is the class membership label ($+1$ for class $+1$ and -1 for class -1) associated with a feature vector $\boldsymbol{x_i}$. Given n such $(\boldsymbol{x_i}, y_i)$ pairs, we would like to learn a linear decision rule $g(\boldsymbol{x})$ that can be used to accurately predict the class label y associated with feature vector $\boldsymbol{x}$.

In C-SVM [Vapnik and Lerner, 1963, Boser et al., 1992, Cortes and Vapnik, 1995], one can think of the linear decision rule g as a means of measuring membership in a particular class. Given a feature vector $\boldsymbol{x}$, C-SVM encourages the function $g(\boldsymbol{x})$ to be positive if $\boldsymbol{x} \in$ class $+1$ and negative if $\boldsymbol{x} \in$ class -1.

We motivate the development of B-SVM in the following way. Suppose that vector $\boldsymbol{x}$ comes from an arbitrary probability distribution $\mathbf{P}_{\boldsymbol{x}}(\boldsymbol{x})$ with mean $\mathbf{E}[\boldsymbol{x}] = \boldsymbol{\mu}$ and finite co-variance $\mathrm{Cov}[\boldsymbol{x}] = \boldsymbol{\Sigma}$. Consider the linear decision rule $g(\boldsymbol{x}) = \boldsymbol{\beta}^T\boldsymbol{x} + \beta_0$. It is easy to see that $g(\boldsymbol{x})$ has mean $\mathbf{E}[g(\boldsymbol{x})] = \boldsymbol{\beta}^T\boldsymbol{\mu} + \beta_0$ and covariance $\mathrm{Cov}[g(\boldsymbol{x})] = \boldsymbol{\beta}^T\boldsymbol{\Sigma}\boldsymbol{\beta}$. By Chebyshev's inequality, there exists a high probability band around $\mathbf{E}[g(\boldsymbol{x})]$ where $g(\boldsymbol{x})$ is expected to lie when $\boldsymbol{x}$ comes from $\mathbf{P}_{\boldsymbol{x}}(\boldsymbol{x})$.

Hence, for every probability distribution of vectors $\boldsymbol{x}$ from class $+1$ and class -1 with finite co-variance, $g(\boldsymbol{x})$ is expected to lie in a certain high probability band. In B-SVM, we choose $g(\boldsymbol{x})$ to encourage:

- ✎ $y\,g(\boldsymbol{x}) > 0$ ☜ same condition as C-SVM
- ✎ $y\,g(\boldsymbol{x}) \in$ certain high probability ***band*** ☜ new B-SVM condition

Both of the above conditions can be satisfied if we encourage:

$$\boxed{y\,g(\boldsymbol{x}) \in [\rho_1, \rho_2] \text{ with } \rho_2 > \rho_1 > 0} \tag{1.1}$$

Since non-linear decision rules in C-SVM are simply linear decision rules operating in a high dimensional space via the kernel trick [Boser et al., 1992], the B-SVM band formation argument holds for non-linear decision rules as well.

2 Problem setup

As per standard SVM terminology, assume that we are given n data-label pairs $(\boldsymbol{x_i}, y_i)$ where $\boldsymbol{x_i}$ are $m \times 1$ vectors and the data labels $y_i \in \{-1, 1\}$. First, we consider only the linear case and afterwards transform to the general case via the kernel trick. Let $m \times 1$ vector $\boldsymbol{\beta}$ and scalar β_0 be parameters of a linear decision rule $g(\boldsymbol{x}) = \boldsymbol{\beta}^T\boldsymbol{x} + \beta_0 = 0$ separating class $+1$ and -1 such that $g(\boldsymbol{x}) > 0$ if $\boldsymbol{x}$ belongs to class $+1$ and vice versa.

2.1 C-SVM objective function

The C-SVM objective function [Cortes and Vapnik, 1995] to be minimized can be written as:

$$f_{CSVM}(\boldsymbol{\beta}, \beta_0) = \frac{1}{2}||\boldsymbol{\beta}||_2^2 + C\sum_{i=1}^{n}[1 - y_i(\boldsymbol{\beta}^T\boldsymbol{x_i} + \beta_0)]_+ \tag{2.1}$$

where $[t]_+$ is the positive part of t:

$$[t]_+ = \begin{cases} 0 & \text{if } t \leq 0, \\ t & \text{if } t > 0. \end{cases} \tag{2.2}$$

and C governs the regularity of the solution. The C-SVM objective function penalizes signed decisions $y_i(\boldsymbol{\beta}^T\boldsymbol{x_i} + \beta_0)$ whenever their value is below 1. This is the only penalty in C-SVM.

2.2 B-SVM objective function

We present below the novel B-SVM objective function that we wish to minimize:

$$f_{BSVM}(\boldsymbol{\beta}, \beta_0) = \frac{1}{2}||\boldsymbol{\beta}||_2^2 + \underbrace{C_1\sum_{i=1}^{n}[\rho_1 - y_i(\boldsymbol{\beta}^T\boldsymbol{x_i} + \beta_0)]_+}_{\text{C-SVM like penalty}} + \underbrace{C_2\sum_{i=1}^{n}[y_i(\boldsymbol{\beta}^T\boldsymbol{x_i} + \beta_0) - \rho_2]_+}_{\text{novel B-SVM penalty}} \tag{2.3}$$

where $\rho_2 > \rho_1 > 0$ are margin parameters specified by the user and C_1 and C_2 are regularization constants. This objective function has two penalty terms:

- The first penalty term is similar to C-SVM. It penalizes signed decisions $y_i(\boldsymbol{\beta}^T\boldsymbol{x_i} + \beta_0)$ whenever their values are below ρ_1 (as opposed to 1 in C-SVM).
- The second penalty term is novel. It penalizes signed decisions $y_i(\boldsymbol{\beta}^T\boldsymbol{x_i} + \beta_0)$ when their values are above ρ_2.

The net effect of these penalty terms is to encourage $y_i(\boldsymbol{\beta}^T\boldsymbol{x_i} + \beta_0)$ to lie in the interval $[\rho_1, \rho_2]$. Please see Figure 1 for a sketch of the two penalty terms in B-SVM.

3 Solving the B-SVM problem

We derive the B-SVM dual problem in order to maximize a lower bound on the B-SVM primal objective function in equation 2.3. This dual problem will be simpler to solve compared to the primal form 2.3. We proceed as follows:

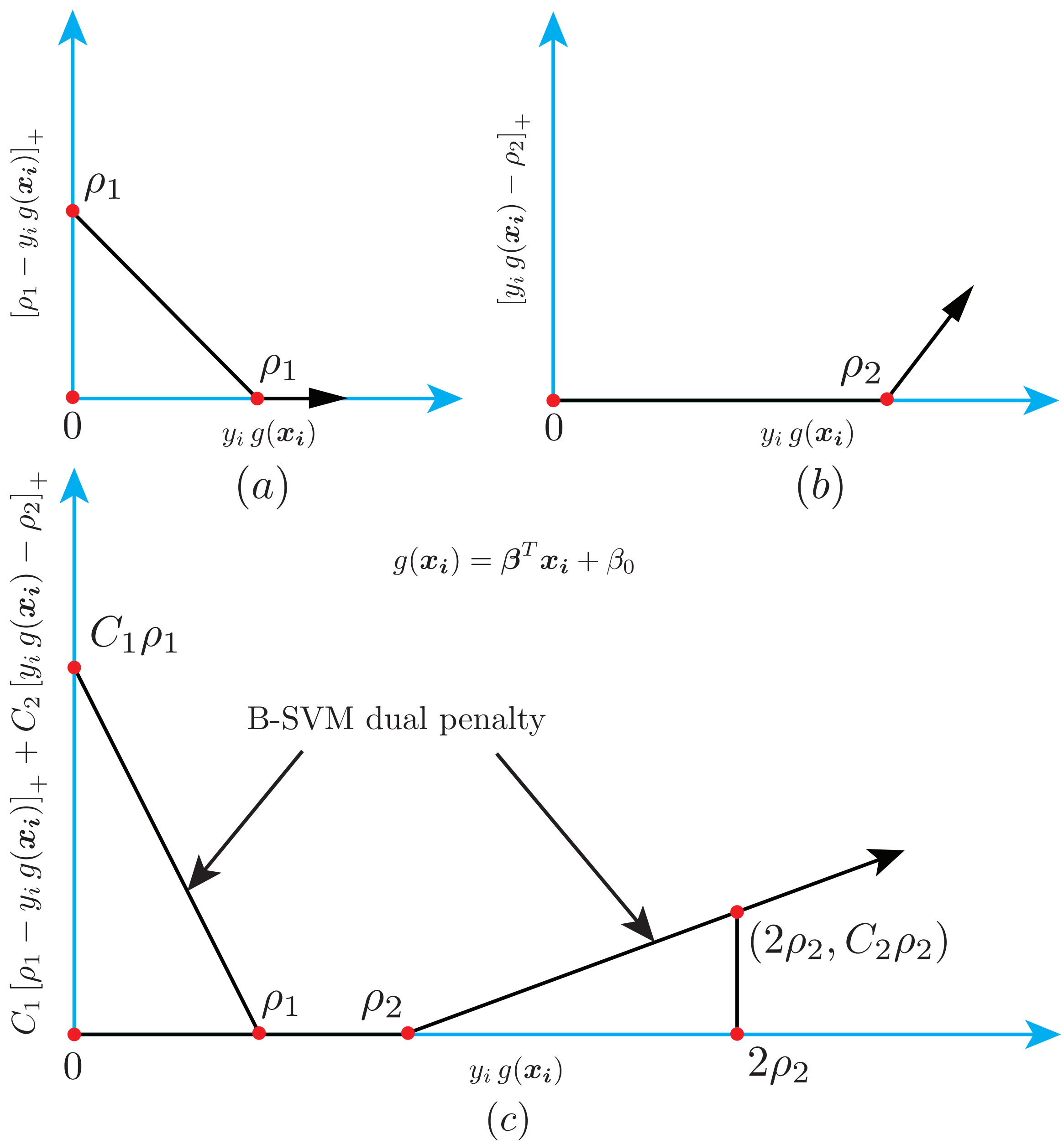


Figure 1: (a) Standard C-SVM like penalty function penalizes $y_i(\boldsymbol{\beta}^T \boldsymbol{x_i} + \beta_0) < \rho_1$. In B-SVM, ρ_1 replaces the constant 1 from C-SVM. (b) Novel B-SVM penalty function. This function penalizes $y_i(\boldsymbol{\beta}^T \boldsymbol{x_i} + \beta_0) > \rho_2$. (c) Total penalty function for B-SVM. If $y_i(\boldsymbol{\beta}^T \boldsymbol{x_i} + \beta_0) \in [\rho_1, \rho_2]$ then the total penalty is 0. Choosing $C_2 < C_1$ will impose a milder penalty for values of $y_i(\boldsymbol{\beta}^T \boldsymbol{x_i} + \beta_0) > \rho_2$.

- As shown in 3.2, the primal problem in 2.3 can be modified into a *strictly* convex objective function with linear inequality constraints using slack variables.
- Consequently, *strong duality* holds and the maximum value of the B-SVM dual objective function is equal to the minimum value of the B-SVM primal objective function in 2.3.

For more details on convex duality, please see Nocedal and Wright [2006].

3.1 The B-SVM dual problem

We introduce slack variables:

$$\begin{aligned} \xi_i &= [\rho_1 - y_i(\boldsymbol{\beta}^T \boldsymbol{x_i} + \beta_0)]_+ \\ \eta_i &= [y_i(\boldsymbol{\beta}^T \boldsymbol{x_i} + \beta_0) - \rho_2]_+ \end{aligned} \tag{3.1}$$

into the primal objective function in 2.3. The modified optimization problem can be written as:

$$\min_{\boldsymbol{\beta},\beta_0,\boldsymbol{\xi},\boldsymbol{\eta}} f_{BSVM}(\boldsymbol{\beta},\beta_0,\boldsymbol{\xi},\boldsymbol{\eta}) = \frac{1}{2}||\boldsymbol{\beta}||_2^2 + C_1\sum_{i=1}^{n}\xi_i + C_2\sum_{i=1}^{n}\eta_i \tag{3.2}$$

$$\begin{aligned} &\xi_i \geq 0 && \text{Lagrange multiplier } \mu_i \\ &\eta_i \geq 0 && \text{Lagrange multiplier } \psi_i \\ &\xi_i \geq \rho_1 - y_i(\boldsymbol{\beta}^T \boldsymbol{x_i} + \beta_0) && \text{Lagrange multiplier } \alpha_i \\ &\eta_i \geq -\rho_2 + y_i(\boldsymbol{\beta}^T \boldsymbol{x_i} + \beta_0) && \text{Lagrange multiplier } \theta_i \end{aligned}$$

After introducing Lagrange multipliers for each inequality constraint as shown in 3.2, the Lagrangian function for problem 3.2 can be written as:

$$\begin{aligned} L(\boldsymbol{\beta},\beta_0,\boldsymbol{\xi},\boldsymbol{\eta},\boldsymbol{\alpha},\boldsymbol{\theta},\boldsymbol{\mu},\boldsymbol{\psi}) = \frac{1}{2}||\boldsymbol{\beta}||_2^2 + C_1\sum_{i=1}^{n}\xi_i + C_2\sum_{i=1}^{n}\eta_i - \sum_{i=1}^{n}\alpha_i\{\xi_i - \rho_1 + y_i(\boldsymbol{\beta}^T \boldsymbol{x_i} + \beta_0)\} \\ - \sum_{i=1}^{n}\theta_i\{\eta_i + \rho_2 - y_i(\boldsymbol{\beta}^T \boldsymbol{x_i} + \beta_0)\} - \sum_{i=1}^{n}\mu_i\xi_i - \sum_{i=1}^{n}\psi_i\eta_i \end{aligned} \tag{3.3}$$

where

$$\alpha_i, \theta_i, \mu_i, \psi_i \geq 0 \tag{3.4}$$

Next, we solve for primal variables $\boldsymbol{\beta}, \beta_0, \boldsymbol{\xi}, \boldsymbol{\eta}$ in terms of the dual variables $\boldsymbol{\alpha}, \boldsymbol{\theta}, \boldsymbol{\mu}, \boldsymbol{\psi}$ by minimizing $L(\boldsymbol{\beta},\beta_0,\boldsymbol{\xi},\boldsymbol{\eta},\boldsymbol{\alpha},\boldsymbol{\theta},\boldsymbol{\mu},\boldsymbol{\psi})$ with respect to the primal variables. Since the Lagrangian in 3.3 is a convex function of the primal variables, its unique global minimum can be obtained using the first order Karush Kuhn Tucker (KKT) conditions given in 3.5 - 3.8:

$$\frac{\partial L}{\partial \boldsymbol{\beta}} = \boldsymbol{\beta} - \sum_{i=1}^{n}\alpha_i y_i \boldsymbol{x_i} + \sum_{i=1}^{n}\theta_i y_i \boldsymbol{x_i} = 0 \tag{3.5}$$

$$\frac{\partial L}{\partial \beta_0} = -\sum_{i=1}^{n} \alpha_i y_i + \sum_{i=1}^{n} \theta_i y_i = 0 \tag{3.6}$$

$$\frac{\partial L}{\partial \xi_l} = C_1 - \alpha_l - \mu_l = 0 \tag{3.7}$$

$$\frac{\partial L}{\partial \eta_l} = C_2 - \theta_l - \psi_l = 0 \tag{3.8}$$

From 3.5, the vector $\boldsymbol{\beta}$ is given by:

$$\boldsymbol{\beta} = \sum_{i=1}^{n} (\alpha_i - \theta_i)\, y_i\, \boldsymbol{x_i} \tag{3.9}$$

From 3.6, vectors $\boldsymbol{\alpha}$ and $\boldsymbol{\theta}$ satisfy the equality constraint:

$$\sum_{i=1}^{n} (\alpha_i - \theta_i)\, y_i = 0 \tag{3.10}$$

Combining 3.7, 3.8 and 3.4, the elements of $\boldsymbol{\alpha}$ must satisfy:

$$0 \leq \alpha_i \leq C_1 \tag{3.11}$$

and elements of $\boldsymbol{\theta}$ satisfy:

$$0 \leq \theta_i \leq C_2 \tag{3.12}$$

Let $\boldsymbol{B}$ be a $n \times n$ matrix with entries:

$$B_{ij} = y_i y_j\, \boldsymbol{x_i}^T \boldsymbol{x_j} \tag{3.13}$$

and $\boldsymbol{e}_n$ be a $n \times 1$ vector of n ones (in MATLAB notation: $\boldsymbol{e}_n$ = `ones(n,1)`). Substituting $\boldsymbol{\beta}$ from 3.9 in 3.3 and noting the constraints 3.7, 3.8 and 3.10, we get the B-SVM dual problem:

$$\boxed{\begin{aligned} \max_{\boldsymbol{\alpha},\boldsymbol{\theta}} L_D(\boldsymbol{\alpha},\boldsymbol{\theta}) = \rho_1\, \boldsymbol{e}_n^T \boldsymbol{\alpha} - \rho_2\, \boldsymbol{e}_n^T \boldsymbol{\theta} - \frac{1}{2}(\boldsymbol{\alpha}-\boldsymbol{\theta})^T \boldsymbol{B}(\boldsymbol{\alpha}-\boldsymbol{\theta}) \\ \mathbf{0} \leq \boldsymbol{\alpha} \leq C_1\, \boldsymbol{e}_n \\ \mathbf{0} \leq \boldsymbol{\theta} \leq C_2\, \boldsymbol{e}_n \\ (\boldsymbol{\alpha}-\boldsymbol{\theta})^T \boldsymbol{y} = 0 \end{aligned}} \tag{3.14}$$

If $C_2 = 0$ and $\rho_1 = 1$ then 3.12 implies $\boldsymbol{\theta} = \mathbf{0}$ and hence we recover the standard C-SVM dual problem.

3.2 Kernelifying B-SVM

Let $\boldsymbol{h}$ be a non-linear vector function that takes inputs $\boldsymbol{x_i}$ into a high dimensional space. Then we recover ***kernel*** B-SVM by doing linear B-SVM on the data-label pairs $(\boldsymbol{h}(\boldsymbol{x_i}), y_i)$ instead of the original pairs $(\boldsymbol{x_i}, y_i)$. In practice, we do not need $\boldsymbol{h}(\boldsymbol{x})$ explicitly but only the dot products through a kernel matrix $\boldsymbol{K}$ with elements:

$$K_{ij} = K(\boldsymbol{x_i}, \boldsymbol{x_j}) = \boldsymbol{h}(\boldsymbol{x_i})^T \boldsymbol{h}(\boldsymbol{x_j}) \tag{3.15}$$

This is the so-called kernel trick. From 3.13, elements of matrix $\boldsymbol{B}$ for transformed feature vectors $\boldsymbol{h}(\boldsymbol{x})$ are given by:

$$B_{ij} = y_i y_j \, \boldsymbol{h}(\boldsymbol{x_i})^T \boldsymbol{h}(\boldsymbol{x_j}) = y_i y_j \, K_{ij} = y_i y_j \, K(\boldsymbol{x_i}, \boldsymbol{x_j}) \tag{3.16}$$

For a new point $\boldsymbol{x}$, the decision rule is then given by:

$$g(\boldsymbol{x}) = \boldsymbol{\beta}^T \boldsymbol{h}(\boldsymbol{x}) + \beta_0 \tag{3.17}$$

and $\boldsymbol{x}$ is classified into class $+1$ if $g(\boldsymbol{x}) > 0$ and into class -1 if $g(\boldsymbol{x}) < 0$. From 3.9, for the transformed feature vectors $\boldsymbol{h}(\boldsymbol{x_i})$, we have:

$$\boldsymbol{\beta} = \sum_{i=1}^{n} (\alpha_i - \theta_i) \, y_i \, \boldsymbol{h}(\boldsymbol{x_i}) \tag{3.18}$$

Using the kernel trick, calculation of $g(\boldsymbol{x})$ does not need $\boldsymbol{h}(\boldsymbol{x})$ explicitly as we can write:

$$\boxed{g(\boldsymbol{x}) = \boldsymbol{\beta}^T \boldsymbol{h}(\boldsymbol{x}) + \beta_0 = \sum_{i=1}^{n} (\alpha_i - \theta_i) \, y_i \, K(\boldsymbol{x_i}, \boldsymbol{x}) + \beta_0} \tag{3.19}$$

Proposition 3.1. *The B-SVM dual objective function $L_D(\boldsymbol{\alpha}, \boldsymbol{\theta})$ in 3.14 is a concave function of $\boldsymbol{\alpha}$ and $\boldsymbol{\theta}$.*

Proof. Since $\boldsymbol{B}$ is symmetric, the Hessian of L_D with respect to the vector $(\boldsymbol{\alpha}, \boldsymbol{\theta})$ is given by:

$$\boldsymbol{H} = \begin{pmatrix} -\boldsymbol{B} & \boldsymbol{B} \\ \boldsymbol{B} & -\boldsymbol{B} \end{pmatrix} \tag{3.20}$$

If $\boldsymbol{c}$ and $\boldsymbol{d}$ are arbitrary $n \times 1$ vectors,

$$\begin{pmatrix} \boldsymbol{c}^T & \boldsymbol{d}^T \end{pmatrix} \boldsymbol{H} \begin{pmatrix} \boldsymbol{c} \\ \boldsymbol{d} \end{pmatrix} = \boldsymbol{c}^T (-\boldsymbol{B}\boldsymbol{c} + \boldsymbol{B}\boldsymbol{d}) + \boldsymbol{d}^T (\boldsymbol{B}\boldsymbol{c} - \boldsymbol{B}\boldsymbol{d}) = -(\boldsymbol{c} - \boldsymbol{d})^T \boldsymbol{B} \, (\boldsymbol{c} - \boldsymbol{d}) \tag{3.21}$$

From 3.16,

$$(\boldsymbol{c} - \boldsymbol{d})^T \boldsymbol{B} \, (\boldsymbol{c} - \boldsymbol{d}) = \sum_{i=1}^{n} \sum_{j=1}^{n} (\boldsymbol{c} - \boldsymbol{d})_i \{y_i y_j \boldsymbol{K}(\boldsymbol{x_i}, \boldsymbol{x_j})\} (\boldsymbol{c} - \boldsymbol{d})_j = \sum_{i=1}^{n} \sum_{j=1}^{n} \{(\boldsymbol{c} - \boldsymbol{d})_i y_i\} \boldsymbol{K}(\boldsymbol{x_i}, \boldsymbol{x_j}) \{(\boldsymbol{c} - \boldsymbol{d})_j y_j\} \tag{3.22}$$

If $\odot$ is an element-wise multiplication operator then:

$$(\boldsymbol{c}-\boldsymbol{d})^T \boldsymbol{B}\,(\boldsymbol{c}-\boldsymbol{d}) = \{(\boldsymbol{c}-\boldsymbol{d}) \odot \boldsymbol{y}\}^T \boldsymbol{K} \{(\boldsymbol{c}-\boldsymbol{d}) \odot \boldsymbol{y}\} \geq 0 \tag{3.23}$$

where the last inequality holds since $\boldsymbol{K}$ is a kernel matrix which is positive definite by 3.15. Therefore, from 3.21 and 3.23:

$$\begin{pmatrix} \boldsymbol{c}^T & \boldsymbol{d}^T \end{pmatrix} \boldsymbol{H} \begin{pmatrix} \boldsymbol{c} \\ \boldsymbol{d} \end{pmatrix} \leq 0 \tag{3.24}$$

for all vectors $\boldsymbol{c}$ and $\boldsymbol{d}$. Thus $L_D(\boldsymbol{\alpha}, \boldsymbol{\theta})$ is a concave function of $(\boldsymbol{\alpha}, \boldsymbol{\theta})$. □ □

It immediately follows that problem 3.14 attempts to maximize a concave function under linear constraints and thus has a unique solution [Nocedal and Wright, 2006].

3.3 Calculation of dual variables

Dual variables $\boldsymbol{\alpha}$, $\boldsymbol{\theta}$, $\boldsymbol{\mu}$, $\boldsymbol{\psi}$ can be calculated as follows:

- Calculation of $\boldsymbol{\alpha}$, $\boldsymbol{\theta}$ requires the solution of a concave maximization problem 3.14 where the elements of $\boldsymbol{B}$ are chosen using a suitable kernel $\boldsymbol{K}(\boldsymbol{x_i}, \boldsymbol{x_j})$. This can be accomplished using an sequential minimal optimization (SMO) type active set technique [Platt, 1998] or a projected conjugate gradient (PCG) technique [Nocedal and Wright, 2006].
- Once $\boldsymbol{\alpha}$ and $\boldsymbol{\theta}$ are known, equations 3.7 and 3.8 give $\boldsymbol{\mu} = C_1 \boldsymbol{e}_n - \boldsymbol{\alpha}$ and $\boldsymbol{\psi} = C_2 \boldsymbol{e}_n - \boldsymbol{\theta}$.

3.4 Calculation of primal variables

Primal variables $\boldsymbol{\beta}$, $\boldsymbol{\beta_0}$, $\boldsymbol{\xi}$, $\boldsymbol{\eta}$ can be calculated as follows:

- $\boldsymbol{\beta}$ is given by equation 3.18.
- Calculation of $\boldsymbol{\beta_0}$, $\boldsymbol{\xi}$, $\boldsymbol{\eta}$ is accomplished by considering the inequality constraints and the KKT *complementarity* constraints for the problem 3.2:

$$\begin{aligned}
&\xi_i \geq 0, \eta_i \geq 0 \\
&\xi_i \geq \rho_1 - y_i \left(\boldsymbol{\beta}^T \boldsymbol{h}(\boldsymbol{x_i}) + \beta_0\right) \\
&\eta_i \geq -\rho_2 + y_i \left(\boldsymbol{\beta}^T \boldsymbol{h}(\boldsymbol{x_i}) + \beta_0\right) \\
&\alpha_i \{\xi_i - \rho_1 + y_i \left(\boldsymbol{\beta}^T \boldsymbol{h}(\boldsymbol{x_i}) + \beta_0\right)\} = 0 \\
&\theta_i \{\eta_i + \rho_2 - y_i \left(\boldsymbol{\beta}^T \boldsymbol{h}(\boldsymbol{x_i}) + \beta_0\right)\} = 0 \\
&\mu_i \xi_i = (C_1 - \alpha_i)\xi_i = 0 \\
&\psi_i \eta_i = (C_2 - \theta_i)\eta_i = 0
\end{aligned} \tag{3.25}$$

Given the positivity constraints 3.4 and the bound constraints 3.11 and 3.12, we consider the following cases:

- If $\alpha_i < C_1$ then $\xi_i = 0$ and similarly if $\theta_i < C_2$ then $\eta_i = 0$.
- If $0 < \alpha_i < C_1$ then we have $\xi_i = 0$ and $\{\xi_i - \rho_1 + y_i(\beta^T x_i + \beta_0)\} = 0$ which can be used to solve for β_0.
- If $0 < \theta_i < C_2$ then we have $\eta_i = 0$ and $\{\eta_i + \rho_2 - y_i \left(\boldsymbol{\beta}^T \boldsymbol{h}(\boldsymbol{x_i}) + \beta_0\right)\} = 0$ which can be used to solve for β_0.
- Similar to C-SVM, for stability purposes we can average the estimate of β_0 over all points where $0 < \alpha_i < C_1$ and $0 < \theta_i < C_2$.
- We can calculate ξ_i for those points for which $\alpha_i = C_1$ using $\xi_i = \rho_1 - y_i \left(\boldsymbol{\beta}^T \boldsymbol{h}(\boldsymbol{x_i}) + \beta_0\right)$.
- Similarly, if $\theta_i = C_2$ then $\eta_i = y_i \left(\boldsymbol{\beta}^T \boldsymbol{h}(\boldsymbol{x_i}) + \beta_0\right) - \rho_2$.

4 Toy data

In order to illustrate the differences between C-SVM and B-SVM we generated artificial data in 2 dimensions as follows:

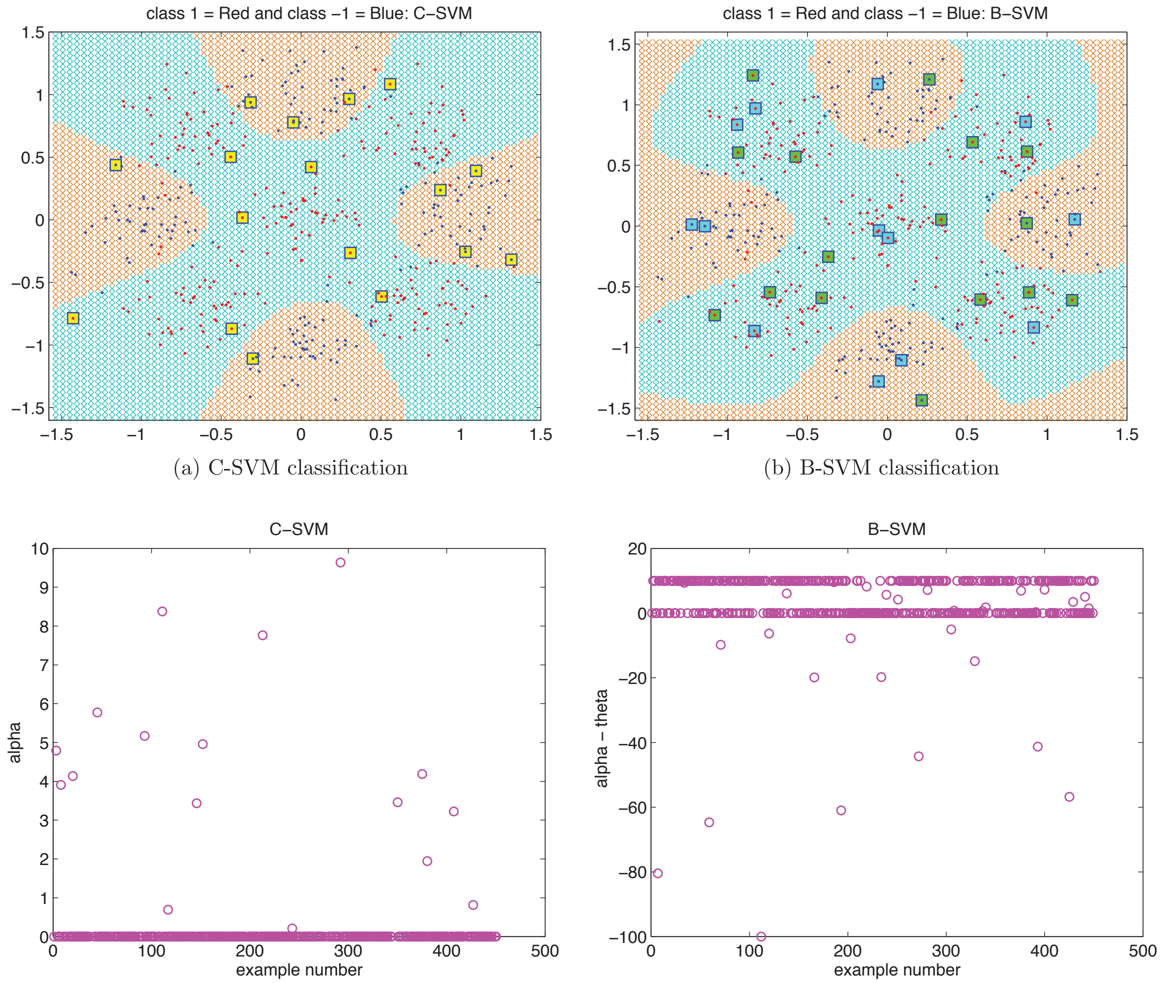
- Class 1 consisted of 5 bivariate Normal clusters centered at $(0, 0)$, $(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}})$, $(\frac{-1}{\sqrt{2}}, \frac{1}{\sqrt{2}})$, $(\frac{-1}{\sqrt{2}}, \frac{-1}{\sqrt{2}})$ and $(\frac{1}{\sqrt{2}}, \frac{-1}{\sqrt{2}})$ and covariance $\sigma_1^2 \boldsymbol{I}_2$ with $\sigma_1 = 0.2$.
- Class -1 consisted of 4 bivariate Normal clusters centered at $(1, 0)$, $(0, 1)$, $(-1, 0)$ and $(0, -1)$ with covariacne $\sigma_2^2 \boldsymbol{I}_2$ with $\sigma_2 = 0.2$.

A radial basis function (RBF) kernel was chosen for computations. For the RBF kernel, the elements of $\boldsymbol{K}$ are given by:

$$K(\boldsymbol{x_i}, \boldsymbol{x_j}) = K_{ij} = \exp\left\{-\gamma\,(\boldsymbol{x_i} - \boldsymbol{x_j})^T\,(\boldsymbol{x_i} - \boldsymbol{x_j})\right\} \tag{4.1}$$

Our parameter settings were as follows:

- For both C-SVM and B-SVM we used the same kernel parameter $\gamma = 1$.
- For C-SVM was used $C = 10$.
- For B-SVM we chose $\rho_1 = 1$ and $C_1 = 10$ (same as C for C-SVM). Thus the parameters of the common penalty term $C_1 \sum_{i=1}^{n} [\rho_1 - y_i(\boldsymbol{\beta}^T \boldsymbol{h}(\boldsymbol{x_i}) + \beta_0)]_+$ are chosen to be identical for C-SVM and B-SVM.
- The parameters of the second penalty term for B-SVM were chosen as $C_2 = 100$ and $\rho_2 = 1.5$. Thus B-SVM will encourage $g(\boldsymbol{x})$ to lie in the interval $[\rho_1, \rho_2] = [1, 1.5]$.



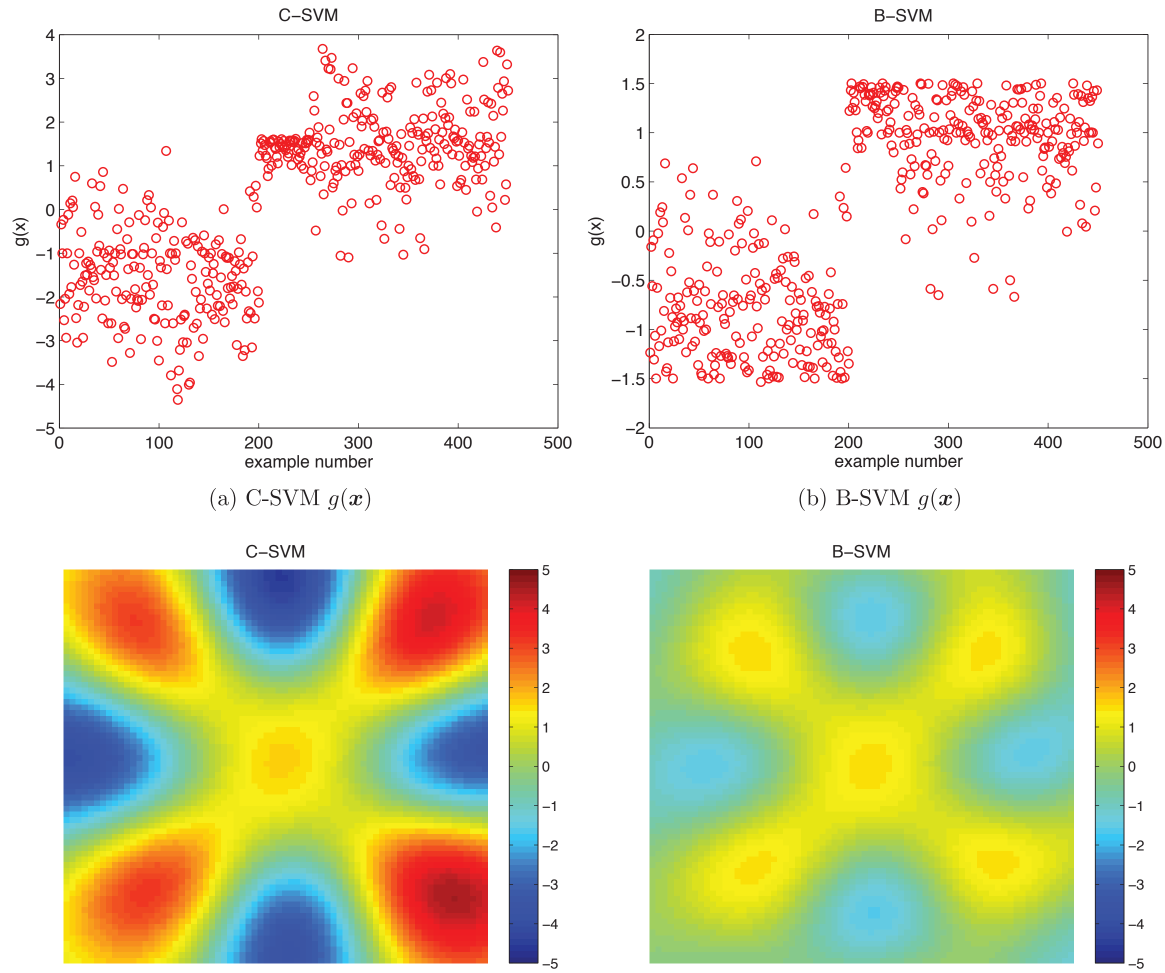
(a) C-SVM classification

(b) B-SVM classification

(c) C-SVM $\boldsymbol{\alpha}$

(d) B-SVM $(\boldsymbol{\alpha} - \boldsymbol{\theta})$

Figure 2: Figure shows classification obtained for example data using (a) C-SVM and (b) B-SVM. Red and Blue points (.) correspond to class $+1$ and -1 respectively. Cyan and Orange x-marks (x) show the C-SVM and B-SVM decision rules evaluated at various points. Class 1 membership is indicated in Cyan and class -1 membership is indicated in Orange. The yellow squares in (a) correspond to support points for which $0 < \alpha_i < C$. The cyan squares in (b) correspond to support points for which $0 < \theta_i < C_2$ and the green squares correspond to support points for which $0 < \alpha_i < C_1$. The sparsity of solution is controlled by $\boldsymbol{\alpha}$ in the case of C-SVM and $(\boldsymbol{\alpha} - \boldsymbol{\theta})$ in the case of B-SVM (c) Shows α_i values for C-SVM. (d) Shows $(\alpha_i - \theta_i)$ values for B-SVM.



(a) C-SVM $g(\boldsymbol{x})$

(b) B-SVM $g(\boldsymbol{x})$

(c) C-SVM $g(\boldsymbol{x})$ heatmap

(d) B-SVM $g(\boldsymbol{x})$ heatmap

Figure 3: Figure shows decision rule $g(\boldsymbol{x})$ for C-SVM (a) and B-SVM (b). Note that in B-SVM the second penalty term $C_2 \sum_{i=1}^{n}[y_i(\boldsymbol{\beta}^T \boldsymbol{h}(\boldsymbol{x_i}) + \beta_0) - \rho_2]_+$ results in most of the $g(\boldsymbol{x})$ values in the interval $[\rho_1, \rho_2] = [1, 1.5]$. (c) Heat map of the decision rule $g(\boldsymbol{x})$ for C-SVM (d) Heat map of the decision rule $g(\boldsymbol{x})$ for B-SVM. In C-SVM the values of decision rule $g(\boldsymbol{x})$ are unbalanced in Class 1. The central cluster located at $(0, 0)$ in Class 1 gets much smaller $g(\boldsymbol{x})$ values in C-SVM than the rest of the Class 1. In B-SVM however, all clusters in Class 1 including the one centered at $(0, 0)$ get similar $g(\boldsymbol{x})$ values. This is a result of the second penalty term in the B-SVM objective function.

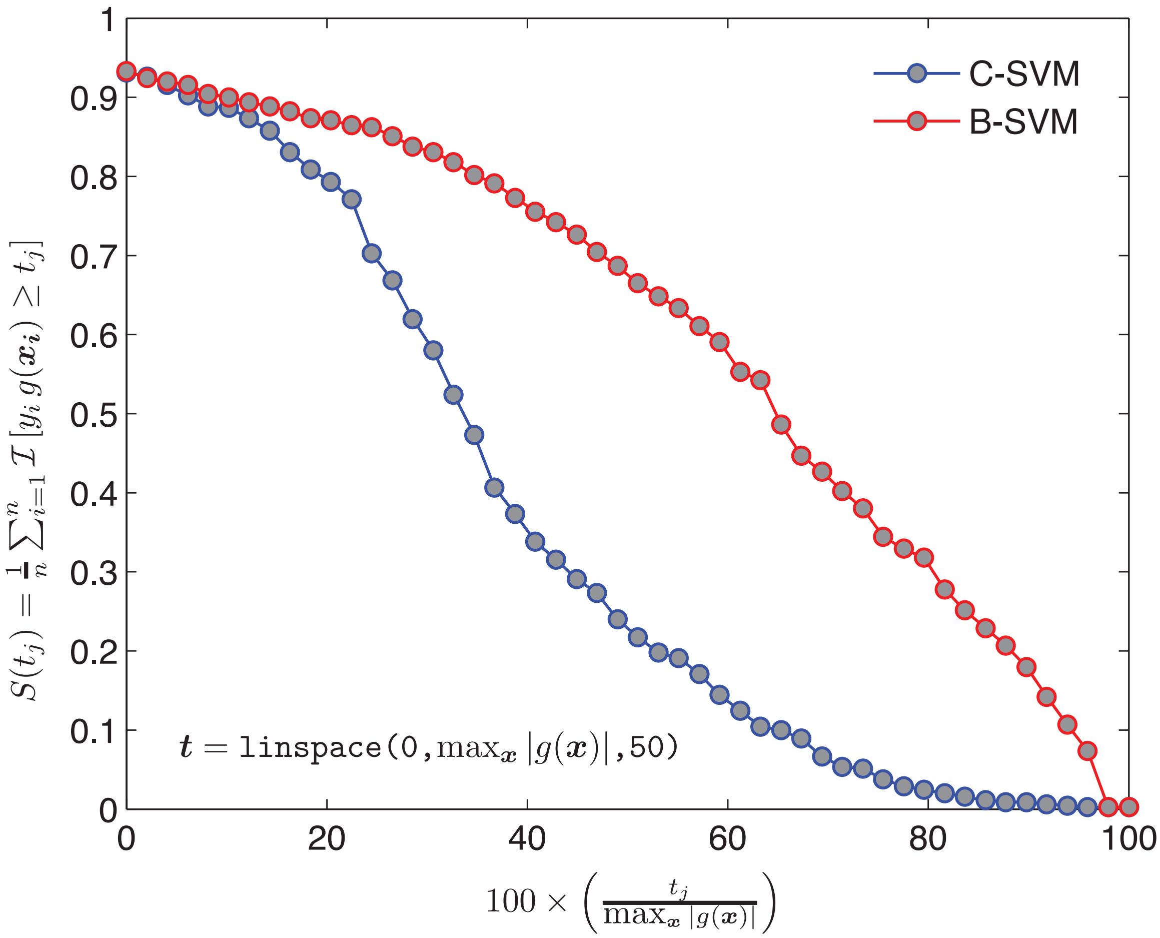


Figure 4: Figure shows the fraction of points classified correctly by both C-SVM (blue curve) and B-SVM (red curve) as a function of the decision rule threshold. The x-axis shows the decision rule threshold as a percentage of the maximum absolute value of the decision function $g(\boldsymbol{x})$ over all training points. The y-axis shows the overall classification accuracy or sensitivity of C-SVM and B-SVM.

Both C-SVM and B-SVM were fitted to the toy data described above. The following differences in the two solutions are noteworthy:

4.1 α-SVs and θ-SVs

The B-SVM dual problem 3.14 contains two variables $\boldsymbol{\alpha}$ and $\boldsymbol{\theta}$. Both α_i and θ_i are positive and satisfy the bound constraints given in 3.14. Therefore, similar to C-SVM, we define 2 types of support vectors (SVs) in B-SVM:

- ✏ Points i for which $\theta_i > 0$ are called the θ-SVs ☜ new SVs that arise in B-SVM
- ✏ Points i for which $\alpha_i > 0$ are called the α-SVs ☜ standard C-SVM like SVs

Figures 2(a) and 2(b) show the C-SVM and B-SVM induced classification respectively for this example problem. Figure 2(b) shows α-SVs for which $0 < \alpha_i < C_1$ and θ-SVs for which $0 < \theta_i < C_2$. It is clear from 3.19 that the sparsity of a B-SVM decision rule depends on the quantities $(\alpha_i - \theta_i)$. Figures 2(c) and 2(d) show a plot of α_i for C-SVM and $(\alpha_i - \theta_i)$ for B-SVM respectively.

4.2 Bounded decision rule

Figures 3(a) and 3(b) show the decision rule values $g(\boldsymbol{x})$ over all training points for C-SVM and B-SVM. Recall that C-SVM does not enforce an upper limit on $g(\boldsymbol{x})$ whereas B-SVM attempts to encourage $g(\boldsymbol{x})$ to lie in $[\rho_1, \rho_2]$. It can be seen in Figure 3(b) that B-SVM was successful in limiting the absolute value of $g(\boldsymbol{x})$ to be $< \rho_2 = 1.5$ with $C_2 = 100$. Figures 3(c) and 3(d) show a heat map of the decision rule for C-SVM and B-SVM respectively evaluated over a 2-D grid containing the training points. It can be seen that:

- ✏ The C-SVM decision rule values are *unbalanced* in class +1 as the central cluster in class +1 gets lower $g(\boldsymbol{x})$ values compared to other clusters in class +1.
- ✏ The decision rule values are *balanced* in class +1 for B-SVM.

4.3 Sensitivity curve

We calculate the quantity:

$$S(t) = \frac{1}{n} \sum_{i=1}^{n} \mathcal{I}\left[y_i \, g(\boldsymbol{x_i}) \geq t\right] \tag{4.2}$$

which is simply the fraction of correctly classified points (or sensitivity) using decision rule $g(\boldsymbol{x})$ at threshold t. To illustrate the variation in sensitivity of C-SVM and B-SVM decision rules:

- For both C-SVM and B-SVM, we divide the range of $g(\boldsymbol{x})$ into 50 equally spaced points as follows (in MATLAB notation):

$$\boldsymbol{t} = \texttt{linspace(0,}\max_{\boldsymbol{x}} |g(\boldsymbol{x})|\texttt{,50)} \tag{4.3}$$

- Then we plot $100 \times \left(\frac{t_j}{\max_{\boldsymbol{x}} |g(\boldsymbol{x})|}\right)$ versus $S(t_j)$.

Figure 4 shows this sensitivity curve. It can be seen that for the same percentage threshold on the decision rule range:

- B-SVM has higher classification accuracy (or is more sensitive) than C-SVM.
- This effect is because of the balanced nature of decision rule values in B-SVM compared to C-SVM (see Figure 3(c) and 3(d)).

5 Discussion and conclusions

In this work, we considered the binary classification problem when the feature vectors in individual classes have finite co-variance. We showed that B-SVM is a natural generalization to C-SVM in this situation. It turns out that the B-SVM dual maximization problem 3.14 retains the concavity property of its C-SVM counterpart and C-SVM turns out to be a special case of B-SVM when $C_2 = 0$. Two types of SVs arise in B-SVM, the α-SVs which are similar to the standard SVs in C-SVM and θ-SVs which arise due to the novel B-SVM objective function penalty 2.3. The B-SVM decision rule is more balanced than the C-SVM decision rule since it assigns $g(\boldsymbol{x})$ values that are comparable in magnitude to different sub-classes (or clusters) of class $+1$ and class -1. In addition, B-SVM retains higher classification accuracy compared to C-SVM as the decision rule threshold is varied from 0 to $\max_{\boldsymbol{x}} |g(\boldsymbol{x})|$. For a training set of size n, B-SVM results in a dual optimization problem of size $2n$ compared to a C-SVM dual problem of size n. Hence it is computationally more expensive to solve a B-SVM problem.

In summary, B-SVM can be used to enforce balanced decision rules in binary classification. It is anticipated that the C-SVM leave one out error bounds for the *bias free* case given in Jaakkola and Haussler [1999] will continue to hold in a similar form for *bias free* B-SVM as well.

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