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# Semi-Supervised Support Vector Machines

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**Kristin P. Bennett\***

Department of Mathematical Sciences  
Rensselaer Polytechnic Institute  
Troy, NY 12180 bennek@rpi.edu

**Ayhan Demiriz**

Department of Decision Sciences and Engineering Systems  
Rensselaer Polytechnic Institute  
Troy, NY 12180 demira@rpi.edu

## Abstract

We introduce a semi-supervised support vector machine ( $S^3VM$ ) method. Given a training set of labeled data and a working set of unlabeled data,  $S^3VM$  constructs a support vector machine using both the training and working sets. We use  $S^3VM$  to solve the overall risk minimization problem (ORM) posed by Vapnik. The ORM problem is to estimate the value of a classification function at the given points in the working set. This contrasts with the standard learning problem of empirical risk minimization (ERM) which estimates the classification function at all possible values. We propose a general  $S^3VM$  model that minimizes both the misclassification error and the function capacity based on all the available data. We show how the  $S^3VM$  model for 1-norm linear support vector machines can be converted to a mixed-integer program (MIP) and then solved exactly using integer programming. Results of  $S^3VM$ -MIP and the standard ERM approach are compared on eleven data sets. Our computational results support the statistical learning theory results showing that incorporating working data improves generalization when insufficient training information is available. In every case,  $S^3VM$  either improved or showed no significant difference in generalization compared to the ERM approach.

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# 1 INTRODUCTION

In this work we propose a method for semi-supervised support vector machines (S<sup>3</sup>VM). S<sup>3</sup>VM are constructed using a mixture of labeled data (the training set) and unlabeled data (the working set). The objective is to assign class labels to the working set such that the “best” support vector machine (SVM) is constructed. If the working set is empty the method becomes the standard SVM approach to classification [20, 9, 8]. If the training set is empty, then the method becomes a form of unsupervised learning. *Semi-supervised* learning occurs when both training and working sets are nonempty. Semi-supervised learning for problems with small training sets and large working sets is a form of semi-supervised clustering. There are successful semi-supervised algorithms for k-means and fuzzy c-means clustering [4, 18]. Clustering is a potential application for S<sup>3</sup>VM as well. When the training set is large relative to the working set, S<sup>3</sup>VM can be viewed as method for solving the *overall risk minimization* (ORM) problem posed by Vapnik at the NIPS 1998 SVM Workshop and in [19, Chapter 10]. S<sup>3</sup>VM for ORM is the focus of this paper.

In classification, the ORM problem is to estimate the class of each given point in the unlabeled working set. The usual support vector machine (SVM) approach, *empirical risk minimization* (ERM), estimates the entire classification function. ORM estimates the classification function value of the working set using information from both the training and working set data. Theoretically, if there is adequate training data to estimate the function satisfactorily, then ERM will be sufficient. We would expect ORM to yield no significant improvement over ERM alone. If, however, there is inadequate training data, then ORM may improve generalization on the working set. Intuitively, we would expect ORM to yield improvements when the training sets are small or when there is a significant deviation between the training and working set subsamples of the total population. Indeed, the theoretical results in [19] support these hypotheses.

In Section 2, we briefly review the standard SVM model for ERM. According to the principles of structural risk minimization, SVM minimize both the empirical misclassification rate and the capacity of the classification function [19, 20]. This is true for both the ERM and ORM approaches. In Section 3, we show how SVM can be extended to the semi-supervised case and how mixed integer programming can be used practically to solve the resulting problem. We compare the ERM and ORM models computationally on eleven problems in Section 4. Our computational results support past theoretical results that improved generalization can be obtained by incorporating working set information during training when there is a deviation between the working set and training set sample distributions. In three of ten real-world problems SVM-MIP achieved a significant increase in generalization. In no case did SVM-MIP ever obtain a significant decrease in generalization. We conclude with a discussion of more general S<sup>3</sup>VM algorithms.

## 2 SVM for Empirical Risk Minimization

The basic ERM task is to estimate a classification function  $f : R^N \rightarrow \{\pm 1\}$  using input-output training data from two classes

$$(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_\ell, y_\ell) \in R^n \times \{\pm 1\}. \quad (1)$$

The function  $f$  should correctly classify unseen examples  $(\mathbf{x}, y)$ , i.e.  $f(\mathbf{x}) = y$  if  $(\mathbf{x}, y)$  is generated from the same underlying probability distribution as the training data. In this work we limit discussion to linear classification functions. We will discuss extensions to the nonlinear case in Section 5. If the points are linearly separable,

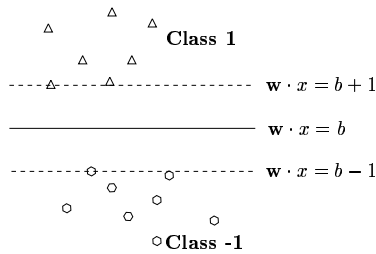


Figure 1: Optimal plane maximizes margin.

then there exist an  $n$ -vector  $\mathbf{w}$  and scalar  $b$  such that

$$\begin{aligned} \mathbf{w} \cdot \mathbf{x}_i - b &\geq 1 & \text{if } y_i = 1, \text{ and} \\ \mathbf{w} \cdot \mathbf{x}_i - b &\leq -1 & \text{if } y_i = -1, i = 1, \dots, \ell \end{aligned} \quad (2)$$

or equivalently

$$y_i[\mathbf{w} \cdot \mathbf{x}_i - b] \geq 1, \quad i = 1, \dots, \ell. \quad (3)$$

The “optimal” separating plane,  $\mathbf{w} \cdot \mathbf{x} = b$ , is the one which is furthest from the closest points in the two classes. Geometrically this is equivalent to maximizing the separation margin or distance between the two parallel planes  $\mathbf{w} \cdot \mathbf{x} = b + 1$  and  $\mathbf{w} \cdot \mathbf{x} = b - 1$  (see Figure 1.)

The “margin of separation” in Euclidean distance is  $2/\|\mathbf{w}\|_2$  where  $\|\mathbf{w}\|_2 = \sum_{i=1}^n \mathbf{w}_i^2$  is the 2-norm. To maximize the margin, we minimize  $\|\mathbf{w}\|_2/2$  subject to the constraints (3). According to structural risk minimization, for a fixed empirical misclassification rate, larger margins should lead to better generalization and prevent overfitting in high-dimensional attribute spaces. The classifier is called a support vector machine because the solution depends only on the points (called support vectors) located on the two supporting planes  $\mathbf{w} \cdot \mathbf{x} = b - 1$  and  $\mathbf{w} \cdot \mathbf{x} = b + 1$ .

In general the classes will not be separable, so the generalized optimal plane (GOP) problem (4) [9, 20] is used. A slack term  $\eta_i$  is added for each point such that if the point is misclassified,  $\eta_i \geq 1$ . The final GOP formulation is:

$$\begin{aligned} \min_{\mathbf{w}, b, \eta} \quad & \sum_{i=1}^{\ell} \eta_i + \frac{1}{2} \|\mathbf{w}\|^2 \\ \text{s.t.} \quad & y_i[\mathbf{w} \cdot \mathbf{x}_i - b] + \eta_i \geq 1 \\ & \eta_i \geq 0, \quad i = 1, \dots, \ell \end{aligned} \quad (4)$$

where  $C > 0$  is a fixed penalty parameter. The capacity control provided by the margin maximization is imperative to achieve good generalization [21, 19].

The Robust Linear Programming (RLP) approach to SVM is identical to GOP except the margin maximization term is changed from the 2-norm  $\|\mathbf{w}\|_2$  to the 1-norm,  $\|\mathbf{w}\|_1 = \sum_{j=1}^n |w_j|$ . The problem becomes the following robust linear program (RLP) [2, 7, 1]:

$$\begin{aligned} \min_{\mathbf{w}, b, s, \eta} \quad & C \sum_{i=1}^{\ell} \eta_i + \sum_{j=1}^n s_j \\ \text{s.t.} \quad & y_i[\mathbf{w} \cdot \mathbf{x}_i - b] + \eta_i \geq 1 \\ & \eta_i \geq 0, \quad i = 1, \dots, \ell \\ & -s_j \leq w_j \leq s_j, \quad j = 1, \dots, n. \end{aligned} \quad (5)$$

The RLP formulation is a useful variation of SVM with some nice characteristics. The 1-norm weight reduction still provides capacity control. The results in [13] can be used to show that minimizing  $\|\mathbf{w}\|_1$  corresponds to maximizing the separation margin using the infinity norm. Statistical learning theory could potentially be extended to incorporate alternative norms. One major benefit of RLP over GOP is dimensionality reduction. Both RLP and GOP minimize the magnitude of the weights  $\mathbf{w}$ . But RLP forces more of the weights to be 0 due to the properties of the 1-norm. Another benefit of RLP over GOP is that it can be solved using linear programming instead of quadratic programming. Both approaches can be extended to handle nonlinear discrimination using kernel functions [8, 12]. Empirical comparisons of the approaches have not found any significant difference in generalization between the formulations [5, 7, 3, 12].

### 3 Semi-supervised support vector machines

To formulate the  $S^3VM$ , we start with either SVM formulation, (4) or (5), and then add two constraints for each point in the working set. One constraint calculates the misclassification error as if the point were in class 1 and the other constraint calculates the misclassification error as if the point were in class  $-1$ . The objective function calculates the minimum of the two possible misclassification errors. The final class of the points corresponds to the one that results in the smallest error. Specifically we define the semi-supervised support vector machine problem ( $S^3VM$ ) as:

$$\begin{aligned} \min_{\mathbf{w}, b, \eta, \xi, z} \quad & C \left[ \sum_{i=1}^{\ell} \eta_i + \sum_{j=\ell}^{\ell+k} \min(\xi_j, z_j) \right] + \|\mathbf{w}\| \\ \text{subject to} \quad & y_i(\mathbf{w} \cdot \mathbf{x}_i + b) + \eta_i \geq 1 \quad \eta_i \geq 0 \quad i = 1, \dots, \ell \\ & \mathbf{w} \cdot \mathbf{x}_j - b + \xi_j \geq 1 \quad \xi_j \geq 0 \quad j = \ell, \dots, \ell + k \\ & -(\mathbf{w} \cdot \mathbf{x}_j - b) + z_j \geq 1 \quad z_j \geq 0 \end{aligned} \quad (6)$$

where  $C > 0$  is a fixed misclassification penalty.

Integer programming can be used to solve this problem. The basic idea is to add a 0 or 1 decision variable,  $d_j$ , for each point  $\mathbf{x}_j$  in the working set. This variable indicates the class of the point. If  $d_j = 1$  then the point is in class 1 and if  $d_j = 0$  then the point is in class  $-1$ . This results in the following mixed integer program ( $S^3VM$ -MIP):

$$\begin{aligned} \min_{\mathbf{w}, b, \eta, \xi, z, d} \quad & C \left[ \sum_{i=1}^{\ell} \eta_i + \sum_{j=\ell}^{\ell+k} (\xi_j + z_j) \right] + \|\mathbf{w}\| \\ \text{subject to} \quad & y_i(\mathbf{w} \cdot \mathbf{x}_i - b) + \eta_i \geq 1 \quad \eta_i \geq 0 \quad i = 1, \dots, \ell \\ & \mathbf{w} \cdot \mathbf{x}_j - b + \xi_j + M(1 - d_j) \geq 1 \quad \xi_j \geq 0 \quad j = \ell, \dots, \ell + k \\ & -(\mathbf{w} \cdot \mathbf{x}_j - b) + z_j + Md_j \geq 1 \quad z_j \geq 0 \quad d_j = \{0, 1\} \end{aligned} \quad (7)$$

The constant  $M > 0$  is chosen sufficiently large such that if  $d_j = 0$  then  $\xi_j = 0$  is feasible for any optimal  $\mathbf{w}$  and  $b$ . Likewise if  $d_j = 1$  then  $z_j = 0$ . A globally optimal solution to this problem can be found using CPLEX or other commercial MIP codes [10] provided computer resources are sufficient for the problem size. Using the mathematical programming modeling language AMPL [11], we were able to express the problem in thirty lines of code plus a data file and solve it using CPLEX.

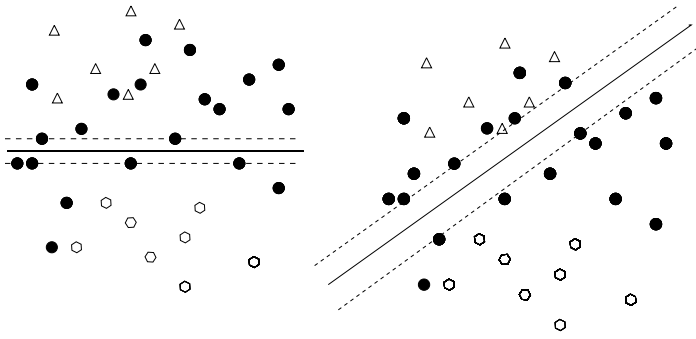


Figure 2: Left = solution found by RLP; Right = solution found by  $S^3VM$ -MIP

## 4 $S^3VM$ and Overall Risk Minimization

The  $S^3VM$ -MIP can be used to solve the Overall Risk Minimization problem. Consider the simple problem given in Figure 20 of [19]. Using RLP alone on the training data results in the separation shown in Figure 1. Figure 2 illustrates what happens when working set data is added. The training set points are shown as transparent circles and hexagons. The working set points are shown as filled circles. The left picture in Figure 2 shows the solution found by RLP. Note that when the working set points are added, the resulting separation has very a small margin. The right picture shows the  $S^3VM$ -MIP solution constructed using the unlabeled working set. Note that a much larger and clearer separation margin is found. These computational solutions are identical to those presented in [19].

We also tested  $S^3VM$ -MIP on ten real-world data sets (eight from [14] and the bright and dim galaxy sets from [15]). There have been many algorithms applied successfully to these problems without incorporate working set information. Thus it was not clear *a priori* that  $S^3VM$  would improve generalization on these data sets. For the data sets where no improvement is possible, we would like ORM to not degrade the performance of the ERM approach. For each data set, we performed 10-fold cross-validation. For the three starred data sets, our integer programming solver failed due to excessive branching required within the CPLEX algorithm. On those data sets we randomly extracted 50 point working sets for each trial. The same  $C$  parameter was used for each data set in both the RLP and  $S^3VM$ -MIP problems<sup>1</sup>. In all ten problems,  $S^3VM$ -MIP never performed significantly worse than RLP. In three of the problems,  $S^3VM$ -MIP performed significantly better. So ORM did not hurt generalization and in some cases it helped significantly. We would expect this based on ORM theory. The generalization bounds for ORM depend on the difference between the training and working sets. If there is little difference, we would not expect any improvement using ORM.

## 5 Conclusion

We introduced a semi-supervised SVM model.  $S^3VM$  constructs a support vector machine using all the available data from both the training and working sets. We show how the  $S^3VM$  model for 1-norm linear support vector machines can be con-

<sup>1</sup>The formula for  $C$  was  $C = \frac{(1-\lambda)}{\lambda(\ell+k)}$  with  $\lambda = .001$ ,  $\ell$  is the size of training set, and  $k$  is the size of the working set.

Table 1: RLP vs S<sup>3</sup>VM-MIP Average Testing Error

Data Set	Dim	Points	CV-size	RLP	S <sup>3</sup> VM-MIP	p-value
Bright	14	2462	50*	0.02	0.018	0.343
Cancer	9	699	70	0.036	0.034	0.591
Cancer(Prognostic)	30	569	57	0.035	0.033	0.678
Dim	14	4192	50*	0.064	0.054	0.096
Heart	13	297	30	0.173	0.160	0.104
Housing	13	506	51	0.155	0.151	0.590
Ionosphere	34	351	35	0.109	0.106	0.59
Musk	166	476	48	0.173	0.173	0.999
Pima	8	769	50*	0.220	0.222	0.678
Sonar	60	208	21	0.281	0.219	0.045

verted to a mixed-integer program (MIP). One great advantage of S<sup>3</sup>VM-MIP is that the globally optimal solution can be found using packages such as CPLEX. Using S<sup>3</sup>VM-MIP we performed an empirical investigation of the ORM problem posed by Vapnik. Our results support the statistical learning theory results that incorporating working data improves generalization when insufficient training information is available. In every case, S<sup>3</sup>VM either improved or showed no significant difference in generalization compared to the usual empirical risk minimization approach. Our empirical results combined with the theoretical results in [19], indicate that ORM constitutes a very promising research direction.

Many research questions remain. Since ORM will be better than the basic ERM approach some of the time, can we identify a priori problems likely to benefit from ORM? The best methods of constructing S<sup>3</sup>VM for the 2-norm case and for nonlinear functions are still open questions. Kernel based methods can be incorporated into S<sup>3</sup>VM. The practical scalability of the approach needs to be explored. We were able to solve moderately-sized problems with on the order of 50 working set points using a general purpose MIP code. The recent success of special purpose algorithms for SVM [16, 17, 6] indicate that such approaches may produce improvement for S<sup>3</sup>VM as well.

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