Class-specific Variable Selection for Multicategory Support Vector Machines

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Abstract

This paper proposes a class-specific variable selection method for multicategory support vector machines (MSVMs). Different from existing variable selection methods for MSVMs, the proposed method not only captures the important variables for classification, but also identifies the discriminable and non discriminable classes so as to enhance the interpretation for multicategory classification problems. Specifically, it minimizes the hinge loss of MSVMs followed by a pairwise fusion penalty. For each variable, this penalty identifies nondiscriminable classes by imposing their associated coefficients in the decision functions to some identical value. Several simulated and real examples demonstrate that the proposed method provides better interpretation through class-specific variable selection while preserving comparable prediction performance with other MSVM methods.

KEY WORDS: Fusion penalty, Lasso, Support vector machine, Variable selection.

1 Introduction

Classification, regression and density function estimation are three canonical problems in machine learning and pattern recognition. In a classification problem, there is a training data set and a test data set. All samples in the training data set are accompanied with the class labels indicating their class membership. The class labels of the samples in the test data set are unobserved. The task of the classification problem is to learn a discrimination rule from the training data and use it to predict the class labels of the test data. In the past decade, support vector machines (SVMs) gained a high degree of attention due to their outstanding prediction performance in real data analysis. The original SVM was proposed by Vapnik (1995) based on the statistical learning theory. Vapnik (1995) also introduced the kernel trick to make SVM have good performance for nonlinear classification problems. The original SVM was designed for a binary classification problem and it was extended to multicategory classification problems in different ways (Vapnik, 1998; Weston and Watkins, 1999; Crammer and Singer, 2001; Lee et al., 2004; Liu and Shen, 2006; Wu and Liu, 2007). The class-specific variable selection method proposed in this paper is based on the MSVM framework proposed by Lee et al. (2004). To clarify the notation, we use SVMs to represent binary SVMs and use MSVMs to represent multicategory SVMs.

Besides the emphasis of prediction performance, in recent years researchers have paid more and more attentions to the interpretability of SVMs. One challenging task of interpretation is how to select the most informative variables for SVM classification. Bradley and Mangasarian (1998) reformulated the standard binary SVM problem into a "loss+penalty" form and demonstrated that the utility of the ℓ_1 penalty can effectively select significant variables by shrinking the small and redundant coefficients to zero. Zhu et al. (2004) provided an efficient algorithm to compute the entire solution path for the ℓ_1 SVM. Under the same framework, other forms of penalties were also studied, such as the ℓ_0 penalty (Weston et al., 2003), the ℓ_q penalty (Liu et al., 2007), the combination of ℓ_0 and ℓ_1 penalties (Liu and Wu, 2007), the elasticnet penalty (Wang et al., 2006), the SCAD penalty (Zhang et al., 2006) and the F_{∞} -norm penalty (Zou and Yuan, 2008). Variable selection for MSVMs is more complex since we need to estimate many decision functions each of which has it own important variables. Wang and Shen (2007) selected informative variables by replacing the ℓ_2 penalty in the standard MSVM (Lee et al., 2004) with an ℓ_1 penalty. Thereafter, Zhang et al. (2008) proposed a supnorm penalty for MSVM. This penalty shrinks all coefficients associated with the same variable simultaneously and hence it tends to produce more sparse solutions than the ℓ_1 MSVM.

All existing variable selection methods for MSVMs select informative variables in a "onein-all-out" manner; that is, a variable is selected if it is important for at least one pair of classes and removed only if it is unimportant for all classes. However, in many practical situations, one may be interested in identifying which variables are important (discriminative) for which specific classes, or in other words, which classes are discriminable for which variables. For example, let's imagine a three-class problem with two variables. The first variable may be important for discriminating classes 1 and 2, but unimportant for classes 2 and 3; on the other hand, the second variable may be important for discriminating classes 1 and 2. We believe that such situations arise often in high-dimensional data, for example, in data obtained from high-throughput expression technologies.

To address this problem, this paper proposes a *class-specific* variable selection method for MSVMs. Specifically, a *pairwise fusion* penalty is introduced to penalize the difference between (all) pairs of coefficients for each variable and shrink the coefficients of nondiscriminable classes to some identical value. If all coefficients associated with a variable are "fused," this variable is regarded as noninformative and removed from the model. Otherwise, the pairwise fusion penalty has the flexibility of only fusing the coefficients of nondiscriminable classes for this variable.

The rest of this article is organized as follows. Section 2 proposes the class-specific variable selection method for MSVMs and introduces a linear programming algorithm to solve the consequent optimization problem; Section 3 and 4 evaluate the performance of the proposed method by two simulated examples and one real example, respectively; and we conclude in Section 5.

2 Methodology

Suppose we observed *n* sample pairs $\{\boldsymbol{x}_i, y_i\}_{i=1}^n$, where $\boldsymbol{x}_i = (x_{i,1}, \ldots, x_{i,p})$ is a vector composed of *p* variables and y_i is the label of \boldsymbol{x}_i . For a *K*-category classification problem, $y_i \in \{1, 2, \ldots, K\}$. Without loss of generality, we assume $\sum_{i=1}^n x_{i,j} = 0$ for all $1 \leq j \leq p$. A multicategory support vector machine aims to learn *K* decision functions $\mathbf{f} = (f_1, \ldots, f_K)$ from the data $\{\boldsymbol{x}_i, y_i\}_{i=1}^n$, where each $f_k(\boldsymbol{x}_i)$, a mapping from the input domain \mathbb{R}^p to \mathbb{R} , represents the strength of the evidence that an example with input \boldsymbol{x}_i belongs to class k. Given an estimate of the decision functions $\hat{\mathbf{f}}$, MSVM assigns a new data point \boldsymbol{x}^* to the class $k^* = \arg \max_{1 \leq k \leq K} f_k(\boldsymbol{x}^*)$.

In linear classification cases, we assume $f_k(\boldsymbol{x}_i) = \boldsymbol{w}_k \boldsymbol{x}_i^{\mathsf{T}} + b_k$, where b_k is the intercept and $\boldsymbol{w}_k = (w_{k,1}, \ldots, w_{k,p})$ is a *p*-dimensional row vector, where each component $w_{k,j}$ captures the contribution of the *j*-th variable to the *k*-th class. All $w'_{k,j}s$ $(1 \le k \le K, 1 \le j \le p)$ are referred as (decision) coefficients and they can be collected in a $K \times p$ matrix (as follows) with rows corresponding to classes and columns to variables

$$\boldsymbol{W} = \begin{bmatrix} w_{1,1} & w_{1,2} & \cdots & w_{1,j} & \cdots & w_{1,p} \\ w_{2,1} & w_{2,2} & \cdots & w_{2,j} & \cdots & w_{2,p} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ w_{K,1} & w_{K,2} & \cdots & w_{K,j} & \cdots & w_{K,p} \end{bmatrix}$$

Throughout the paper, we use \boldsymbol{w}_k to represent the coefficients associated with the k-th class (k-th row vector of \boldsymbol{W}) and use $\boldsymbol{w}_{(j)} = (w_{1,j}, \ldots, w_{K,j})^{\mathsf{T}}$ to represent the coefficients for the

j-th variable (*j*-th column vector of \boldsymbol{W}).

In this paper, we focus on a family of MSVM methods based on the following "Loss+Penalty" framework

$$\min_{\boldsymbol{b},\boldsymbol{W}} \sum_{i=1}^{n} \sum_{k=1}^{K} \mathbb{I}(y_i \neq k) [b_k + \boldsymbol{w}_k^{\mathsf{T}} \boldsymbol{x}_i + 1]_+ + \mathcal{J}_{\lambda}(\boldsymbol{W})$$

subject to
$$\sum_{k=1}^{K} b_k = 0, \quad \sum_{k=1}^{K} w_{k,j} = 0, \quad 1 \le j \le p.$$
(1)

where $\mathbf{b} = (b_1, \dots, b_K)^{\mathsf{T}}$ is the vector of intercepts and $\mathbb{I}(y_i \neq k)$ is an indicator function with value 1 if $y_i \neq k$ and 0 otherwise. The sum-to-zeros constraints $\sum_{k=1}^{K} b_k = 0$ and $\sum_{k=1}^{K} w_{k,j} = 0$ impose the identifiability of the solution and they are also the necessary conditions for the Fisher consistency of the MSVM (Lee et al., 2004). $J_{\lambda}(\mathbf{W})$ is a penalty function with tuning parameter λ . It involves some prior information to help estimate the coefficients in \mathbf{W} . For example, the standard MSVM (Lee et al., 2004) employs an ℓ_2 penalty as follows

$$\mathbf{J}_{\lambda}^{L2}(\boldsymbol{W}) = \lambda \sum_{j=1}^{p} \sum_{k=1}^{K} w_{k,j}^{2}$$

$$\tag{2}$$

For the purpose of variable selection, Wang and Shen (2007) proposed to use the ℓ_1 penalty as follows

$$\mathbf{J}_{\lambda}^{L1}(\boldsymbol{W}) = \lambda \sum_{j=1}^{p} \sum_{k=1}^{K} \tau_{k,j} |w_{k,j}|$$
(3)

where $\tau_{k,j}$ is the adaptive weight defined as $\tau_{k,j} = 1/|\tilde{w}_{k,j}|$. Due to its singularity property, the ℓ_1 penalty shrinks some $w_{k,j}$'s to be exactly zero and removes the *j*-th variable from the model if all coefficients associated with the *j*-th variable (i.e., $w_{k,j}$ for all $1 \le k \le K$) are shrunken to zero (in this case, the *j*-th variable does not contribute to discriminating between the decision functions f_1, \ldots, f_K and thus it is a *noninformative* variable). Zhang et al. (2008) proposed a supnorm (ℓ_{∞}) penalty (as follows) to remove the insignificant variables more

efficiently.

$$\mathbf{J}_{\lambda}^{SN}(\boldsymbol{W}) = \lambda \sum_{j=1}^{p} \|\boldsymbol{w}_{(j)}\|_{\infty} = \lambda \sum_{j=1}^{p} \max_{1 \le k \le K} \tau_{k,j} |w_{k,j}|$$
(4)

This penalty treats all coefficients associated with the same variable as a natural group and shrinks them to zero simultaneously. It should be noted that the ℓ_1 penalty usually tends to shrink only some $w_{k,j}$'s to zero, thus being more flexible but less efficient in removing noninformative variables. In Zhang et al. (2008), the adaptive weights $\tau_{k,j}$, $1 \le k \le K, 1 \le$ $j \le p$ are defined in two ways: (1) $\tau_{k,j} = 1/|\tilde{w}_{k,j}|, 1 \le k \le K, 1 \le j \le p$; (2) $\tau_{1,j} = \cdots =$ $\tau_{K,j} = 1/\max\{|\tilde{w}_{1,j}|, \ldots, |\tilde{w}_{K,j}|\}, 1 \le j \le p$.

2.1 Class-specific Variable Selection

Given our focus on class-specific variable selection introduced in Section 1, we propose the following *pairwise fusion penalty* for MSVM

$$\mathbf{J}^{PF}(\boldsymbol{W}) = \sum_{j=1}^{p} \sum_{1 \le k < k' \le K} \tau_{k,k'}^{(j)} |w_{k,j} - w_{k',j}|$$
(5)

For each variable, this penalty aims at shrinking the differences between the coefficients associated with every pair of classes. Due to the singularity of the absolute value function, some terms in the sum are shrunken to exactly zero, resulting in some coefficients $w_{k,j}$'s having identical values. For example, if coefficients $w_{k,j} = w_{k',j}$, then $f_k(\mathbf{x}) - f_{k'}(\mathbf{x})$ doesn't depend on the *j*-th variable. Consequently, this variable is considered to be unimportant for discriminating between class k and k', though it may be important for separating other classes. Moreover, if all coefficients for the same variable are shrunken to the same value, then this variable doesn't help discriminate between the decision functions f_1, \ldots, f_K and can be removed from the model. We refer this variable as a noninformative variable. For a two-class problem, the pairwise fusion penalty proposed here is equivalent to the ℓ_1 penalty under the constraint $\sum_{k=1}^{K} w_{k,j} = 0$ $(1 \le j \le p)$. Here we set the adaptive weights $\tau_{k,k'}^{(j)}$. based on the intuition: if variable j is important for separating classes k and k', we would like the corresponding $\tau_{k,k'}^{(j)}$ to be small, thus the difference between $w_{k,j}$ and $w_{k',j}$ is lightly penalized. On the other hand, if variable j is unimportant for separating clusters k and k', we would like the corresponding $\tau_{k,k'}^{(j)}$ to be large, hence the difference between $w_{k,j}$ and $w_{k',j}$ is heavily penalized. In our implementation, we compute the weights using the estimates from standard MSVM, i.e., $\tau_{k,k'}^{(j)} = 1/|\tilde{w}_{k,j} - \tilde{w}_{k',j}|$ where $\tilde{w}_{k,j}$ is the estimate of $w_{k,j}$ by solving (1) with penalty (2). Note that this decomposition has also been used by Guo et al. (2010) for clustering purpose.

2.2 Algorithm

Here we discuss how to minimize objective function (1) with penalty (5), i.e., the optimization problem as follows

$$\min_{b,W} \sum_{i=1}^{n} \sum_{k=1}^{K} \mathbb{I}(y_i \neq k) [b_k + w_k^T x_i + 1]_+ \\
+ \lambda \sum_{j=1}^{p} \sum_{1 \le k < k' \le K} \tau_{k,k'}^{(j)} |w_{k,j} - w_{k',j}| \\
\text{subject to} \sum_{k=1}^{K} b_k = 0, \sum_{k=1}^{K} w_{k,j} = 0, \quad 1 \le j \le p$$
(6)

Objective function (6) can be converted to a standard linear programming (LP) problem and solved by most linear programming software. Specifically, denote $a_{i,k} = \mathbb{I}(y_i \neq k)$, $\xi_{i,k} = [b_k + w_k^T x_i + 1]_+$ and $\theta_{k,k',j} = w_{k,j} - w_{k',j}$. To deal with the absolute value in (6), let $\theta_{k,k',j}^+ = \max\{0, \theta_{k,k',j}\}$ be the positive part of $\theta_{k,k',j}$ and $\theta_{k,k',j}^- = \max\{0, -\theta_{k,k',j}\}$ be the negative part of $\theta_{k,k',j}$. Consequently, $\theta_{k,k',j} = \theta_{k,k',j}^+ - \theta_{k,k',j}^-$ and $|\theta_{k,k',j}| = \theta_{k,k',j}^+ + \theta_{k,k',j}^-$. Thus, (6) can be written as

$$\begin{array}{ll}
\underset{k=1}{\min} & \sum_{i=1}^{n} \sum_{k=1}^{K} a_{i,k} \xi_{i,k} \\
& + \lambda \sum_{j=1}^{p} \sum_{1 \leq k < k' \leq K} \tau_{k,k'}^{(j)} (\theta_{k,k',j}^{+} + \theta_{k,k',j}^{-}) \\
\text{subject to} & \xi_{i,k} \geq b_k + w_k^T x_i + 1, \quad \xi_{i,k} \geq 0, \\
& \text{for all } 1 \leq i \leq n, \quad 1 \leq k \leq K; \\
& \sum_{k=1}^{K} b_k = 0, \quad \sum_{k=1}^{K} w_{k,j} = 0, \\
& \text{for all } 1 \leq j \leq p; \\
& \theta_{k,k',j}^{+} - \theta_{k,k',j}^{-} = w_{k,j} - w_{k',j}, \\
& \text{for all } 1 \leq k < k' \leq K, \quad 1 \leq j \leq p. \\
\end{array}$$
(7)

where $\Theta = \{\theta_{k,k',j}^+, \theta_{k,k',j}^- : 1 \le k < k' \le K, 1 \le j \le p\}$ and $\boldsymbol{\xi} = (\xi_{i,k})_{n \times K}$. In this article, objective function (7) was solved by the mathematical programming language AMPL with linear programming package CPLEX.

3 Simulation Study

In this section, we illustrate the performance of the proposed class-specific variable selection method on two synthetic examples with four and five classes, respectively. We compare four different MSVM methods, pairing it with: the ℓ_1 penalty ("L1", equation (3)), two supnorm penalties ("SN-I" and "SN-II", equation (4) with two types of adaptive weights), the proposed pairwise fusion penalty ("PF", equation (5)). In each simulation, 50 training observations, 50 validation observations and 10,000 test observations are generated from each class. The tuning parameter λ is selected on the validation set via a grid $\{2^{-15}, 2^{-14}, \ldots, 2^{15}\}$. We repeat this procedure 100 times for each simulation and record the average test error rates as compared to the true class labels, and average selection rate for both informative and noninformative variables.

Example 1

In this simulation, there are four classes and p = 10 variables, with the first two variables being informative and the remaining ones noninformative. The variables were generated according to the following mechanism: the two informative variables x_1 and x_2 are independently uniformly distributed in [-1, 1], whereas the remaining eight noninformative variables are all *i.i.d.* $N(0, 8^2)$. Denote $\boldsymbol{x} = (x_1, \ldots, x_{10})$, then we define the decision function for the *k*-th class as follows

$$\mathbf{f}_k(x) = \begin{cases} 10x_1 + 5x_2, & \text{if } k = 1; \\ 5x_2, & \text{if } k = 2; \\ -5x_2, & \text{if } k = 3; \\ -10x_1 - 5x_2, & \text{if } k = 4. \end{cases}$$

and we assign \boldsymbol{x} to class k with a probability proportional to $\exp\{f_k(\boldsymbol{x})\}$. In this example, x_1 is unimportant for discriminating between classes 2 and 3 and x_2 is unimportant for discriminating between classes 1 and 2 and classes 3 and 4.

Table 1: Simulation results for Example 1. "Error rate" is the proportion of wrongly classified samples in the test data set. "Info" is the number of selected informative variables (out of 2 for Example 1 and out of 3 for Example 2). "Noninfo" is the number of noninformative variables (out of 8 for Example 1 and out of 7 for Example 2). All results are averaged over 100 replications and their corresponding standard deviations are recorded in the parentheses.

Example	Method	Error rate	Info	Noninfo
	L1	0.142(0.009)	2(0)	0.980(1.301)
1	SN-I	0.137(0.006)	2(0)	$0.280\ (0.573)$
1	SN-II	$0.141 \ (0.009)$	2(0)	0.900(1.919)
	\mathbf{PF}	$0.136\ (0.004)$	2(0)	$0.040\ (0.198)$
	L1	0.176(0.014)	3(0)	1.960(1.761)
2	SN-I	$0.191 \ (0.016)$	3(0)	2.240(2.200)
Ζ	SN-II	0.168(0.014)	3(0)	0.240(0.476)
	\mathbf{PF}	$0.171 \ (0.022)$	3(0)	$0.040\ (0.198)$

Example 2

In this example, a five-class scenario is considered. There are a total of p = 10 variables with the first three informative and the other seven noninformative. Similar to Example 1, the informative variables are independently uniformly distributed in [-1, 1], whereas the seven noninformative variables are all *i.i.d.* $N(0, 8^2)$. We define the decision function for the k-the class as

$$\mathbf{f}_{k}(\boldsymbol{x}) = \begin{cases} 4x_{1} - 10x_{2} + 6x_{3}, & \text{if } k = 1; \\ 4x_{1} + x_{3}, & \text{if } k = 2; \\ -x_{1} + x_{3}, & \text{if } k = 3; \\ -x_{1} - 4x_{3}, & \text{if } k = 4; \\ -6x_{1} + 10x_{2} - 4x_{3}, & \text{if } k = 5. \end{cases}$$

and assign \boldsymbol{x} to class k with a probability proportional to $\exp\{f_k(\boldsymbol{x})\}$. Notice that x_1 is unimportant for discriminating between classes 1 and 2 and classes 3 and 4; x_2 is unimportant for classes 2, 3 and 4; and x_3 is unimportant for classes 2 and 3 and classes 4 and 5.

Example	Variable	Pair	L1	SN-I	SN-II	PF
	1	2/3	0.08	0.00	0.00	0.34
1	2	1/2	0.00	0.52	0.00	0.96
	2	3/4	0.00	0.52	0.00	0.94
	1	1/2	0.00	0.06	0.00	0.78
	1	3/4	0.66	0.00	0.00	0.94
		2/3	0.36	0.00	0.00	0.72
2	2	2/4	0.08	0.00	0.00	0.50
		3/4	0.22	0.00	0.00	0.76
	3	2/3	0.62	0.00	0.00	0.88
	J	4/5	0.00	0.16	0.00	0.74

Table 2: Results of class-specific variable selection for nondiscriminable class pairs.

The results over 100 replications for both simulation scenarios are summarized in Table 1. All methods are able to identify the informative variables. Compared with L1, SN-I and SN-II, the proposed PF penalty is more effective at removing noninformative variables and produces lower or comparable prediction error rates.

If a variable is unimportant for separating a pair of classes, and the corresponding estimated coefficients are also the same, we consider this as a correct "fusion". Table 2 summarizes these results. Specifically, each row in the table gives the proportion of correctly fused variables (averaged over 100 replications) that are noninformative for separating the corresponding pair of classes (indicated in column "Pair"). For example, the second row shows that for the PF method, on average 96% of the first two informative variables are correctly fused for classes 1 and 2. It is also clear that PF dominates other methods in terms of correctly fusing the coefficients of nondiscriminable classes. It should also be pointed out that although L1 and SN-I correctly fuse some coefficients of nondiscriminable classes, e.g., in the first row (L1) as well as in the second and third row (SN-I), the result is an artifact. In Example 1, the coefficients of classes 2 and 3 for variable 1 are all equal to zero, which happens to be the value that the ℓ_1 penalty shrinks to. The same reasoning applies to classes 2, 3 and 4 for variable 2 in Example 2 (row 6–8, column "L1"). On the other hand, in Example 1, although classes 1 and 2 (as well as classes 3 and 4) have the same coefficient for variable 2, the L1 method fails to fuse them, since their coefficients are different from zero. In contrast to L1, SN-I tends to encourage the coefficients with large magnitudes to have some identical values. In Example 1, for instance, the coefficients of classes 1 and 2 (as well as those of classes 3 and 4) for variable 2 have the same value with large magnitude, thus they are identified by SN-I. On the other hand, it fails to fuse classes 2 and 3 for variable 1, since their coefficients are close to zero. However, the PF method identifies the structure correctly in both situations.

4 Real Data Analysis

4.1 Microarray Example

In this example, we apply the proposed pairwise fusion SVM method to conduct classspecific variable selection on a microarray dataset of small round blue cell tumors (SRBCT) of childhood cancer (Khan et al., 2001). This dataset contains the expression profiles of 2308 genes obtained from 83 tissue samples, 53 of which belong to the training set and the remaining 30 belonging to the test set. These subjects are classified into four tumor subtypes: Ewing family of tumors (EWS), rhabdomyosarcoma (RMS), neuroblastoma (NB) and Burkitt lymphoma (BL). We preprocessed the data by selecting a subset of 500 genes according to their marginal relevance criterion (Dudoit et al., 2002; Zhang et al., 2008):

$$R_{j} = \frac{\sum_{i=1}^{n} \sum_{k=1}^{K} \mathbb{I}(y_{i} = k)(\mu_{k,j} - \mu_{j})}{\sum_{i=1}^{n} \sum_{k=1}^{K} \mathbb{I}(y_{i} = k)(x_{i,j} - \mu_{k,j})}$$
(8)

where $\mu_{k,j}$ is the mean of all samples in class k and variable j and μ_j is the mean of all samples in variable j. The term on the numerator reflects the between-class distance and the term on the denominator reflects the within-class distance. Therefore, this criterion gives large values to those genes expressing heterogeneously across the classes and homogenously within the classes. The top 500 genes are collected and the new data are centered and scaled along each variable before classification.

All MSVM methods with different penalties are applied to the training set and the tuning parameter λ is selected by five-fold cross validation. The prediction results on the test data are summarized in Table 3. All these methods produce similar test error rates and select similar number of genes.

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	Method	Test Error $(\%)$	Selected Genes $(\#)$	
	L1	0	32	
	SN-I	3.3	29	
	SN-II	0	35	
	\mathbf{PF}	0	32	

Table 3: Classification and variable selection results of SRBCT data set.

Figure 1 shows the results for class-specific variable selection. The rows correspond to the 32 (out of the 500) genes selected by the PF method and the column to the six pairs formed from the four subtypes. A black (white) spot indicates that the estimated coefficients of the corresponding gene for the two subtypes are different (the same). For example, gene "1358266" is unimportant for discriminating subtypes EWS, NB and BL. We can see that PF provides a more informative way for describing the functions of a gene with respect to discriminating different tumor subtypes.

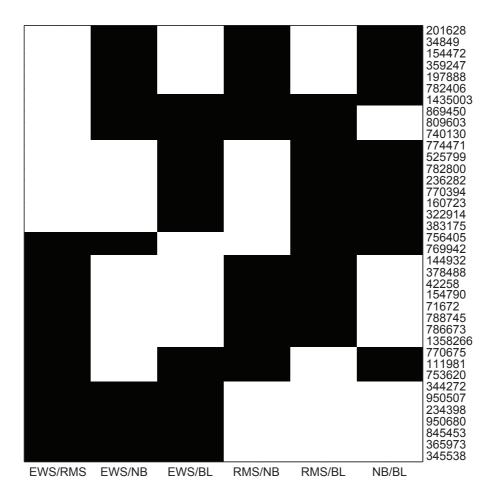


Figure 1: Results of class-specific variable selection for the PF method on the SRBCT data. Each row corresponds to a gene (denoted by its ID). Each column corresponds to a pair of tumor subtypes; for example, "EWS/NB" indicates subtypes EWS and NB. A black (white) spot indicates that the estimated coefficients of the corresponding gene for the two subtypes are different (the same).

4.2 Web Mining Example

The data set comes from the World Wide Knowledge Base project at Carnegie Mellon University. It was collected in 1997 and includes webpages from websites at computer science departments in the following four universities: Cornell, Texas, Washington, and Wisconsin. The webpages were manually classified into seven categories, but in this example, only 1396 webpages corresponding to the four largest categories were used: student (544 webpages), faculty (374 webpages), course (310 webpages) and project (168 webpages). The original data set was preprocessed by Cardoso-Cachopo (2009) following the following steps: (1) Substituting space for tab, newline, and return characters; (2) Keeping only letters (that is, turning punctuation, numbers, etc. into spaces) and turning all letters to lowercase; (3) Removing words less than 3 characters long and removing the 524 smart stopwords; (4) Substituting a single space for multiple spaces; (5) Stemming the documents by applying a stemmer algorithm (Porter, 1980) to the remaining text.

The log-entropy weighting method (Dumais, 1991) was used to calculate the termdocument matrix $\mathbf{X} = (x_{i,j})_{n \times p}$, with n and p denoting the number of webpages and distinct terms, respectively. Let $f_{i,j}$, $1 \le i \le n, 1 \le j \le p$ be the number of times the j-th term appears in the *i*-th webpage and let $p_{i,j} = f_{i,j} / \sum_{i=1}^{n} f_{i,j}$. Then, the log-entropy weight of the j-th term is defined as

$$e_j = 1 + \sum_{i=1}^n p_{i,j} \log(p_{i,j}) / \log(n)$$
.

Finally, the term-document matrix \boldsymbol{X} is defined as

$$x_{i,j} = e_j \log(1 + f_{i,j}) , 1 \le i \le n , \ 1 \le j \le p ,$$

and it is normalized along each column. We applied the proposed method to n = 1396 documents in the four largest categories and p = 100 terms with the highest log-entropy weights out of a total of 4800 terms.

Table 4 shows the prediction and variable selection results. Again, all these methods produce similar test error rates and select similar number of variables (terms). Figure 2 illustrates the results of class-specific variable selection. We can see that many terms only contribute to discriminate a set of topics. For example, the topics "faculty", "course" and "project" can not be discriminated by terms "work", "member" etc. Therefore, class-specific variable selection provides better interpretation and it helps deeper understand the structure of the data.

Method	l Test Error $(\%)$	Selected Terms $(\#)$
L1	22.6	81
SN-I	23.5	80
SN-II	23.0	74
\mathbf{PF}	23.3	84

Table 4: Classification and variable selection results of web mining data set using top 100 terms.

5 Conclusion

We have developed a method for simultaneously classifying high-dimensional data and selecting informative variables, by employing a penalized multicategory support vector machine framework. In particular, the proposed method penalizes the difference between the coefficients for each pair of classes and for each variable, which allows one to identify and remove unimportant variables for selected subsets of classes. This allows one to gain more insight into the function of particular variables and potentially discover heterogeneous structures that other available methods are unable to capture.

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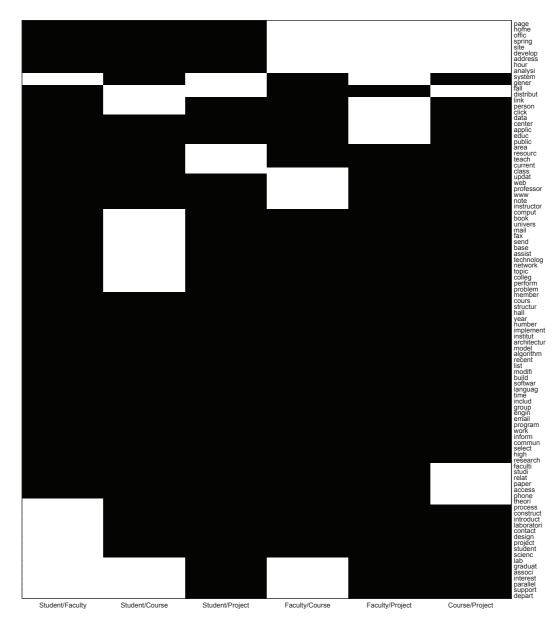


Figure 2: Results of class-specific variable selection for the PF method on the web mining data. Each row corresponds to a term and each column corresponds to a pair of topics. A black (white) spot indicates that the the corresponding terms is discriminable (nondiscriminable) for the associated two topics.