Combining SVMs with Various Feature Selection Strategies

Yi-Wei Chen and Chih-Jen Lin

Department of Computer Science, National Taiwan University, Taipei 106, Taiwan

Summary. This article investigates the performance of combining support vector machines (SVM) and various feature selection strategies. Some of them are filter-type approaches: general feature selection methods independent of SVM, and some are wrapper-type methods: modifications of SVM which can be used to select features. We apply these strategies while participating at NIPS 2003 Feature Selection Challenge and rank third as a group.

1 Introduction

Support Vector Machine (SVM) (Boser et al. 1992; Cortes and Vapnik 1995) is an effective classification method, but it does not directly obtain the feature importance. In this article we combine SVM with various feature selection strategies and investigate their performance. Some of them are "filters": general feature selection methods independent of SVM. That is, these methods select important features first and then SVM is applied for classification. On the other hand, some are wrapper-type methods: modifications of SVM which choose important features as well as conduct training/testing. We apply these strategies while participating at NIPS 2003 Feature Selection Challenge. Overall we rank third as a group and are the winner of one data set.

In NIPS 2003 Feature Selection Challenge, the main judging criterion is the balanced error rate (BER). Its definition is:

$$\begin{aligned}\text{BER} \equiv \frac{1}{2}\Big(&\frac{\text{\# positive instances predicted wrong}}{\text{\# positive instances}} + \\ &\frac{\text{\# negative instances predicted wrong}}{\text{\# negative instances}}\Big)\,.\end{aligned} \tag{1}$$

For example, assume a test data set contains 90 positive and 10 negative instances. If all instances are predicted as positive, then BER is 50% since the first term of (1) is 0/90 but the second is 10/10. There are other judging criteria such as the number of features and probes, but throughout the competition we focus on how to get the smallest BER.

This article is organized as follows. In Section 2 we introduce support vector classification. Section 3 discusses various feature selection strategies. In Section 4, we show the experimental results during the development period of the competition. In Section 5, the final competition results are listed. Finally, we have discussion and conclusions in Section 6. All competition data sets are available at `http://clopinet.com/isabelle/Projects/NIPS2003/`.

2 Support Vector Classification

Recently, support vector machines (SVMs) have been a promising tool for data classification. Its basic idea is to map data into a high dimensional space and find a separating hyperplane with the maximal margin. Given training vectors $\boldsymbol{x}_k \in R^n, k = 1, \ldots, m$ in two classes, and a vector of labels $\boldsymbol{y} \in R^m$ such that $y_k \in \{1, -1\}$, SVM solves a quadratic optimization problem:

$$\begin{aligned} \min_{\boldsymbol{w}, b, \boldsymbol{\xi}} \quad & \frac{1}{2}\boldsymbol{w}^T\boldsymbol{w} + C\sum_{k=1}^{m} \xi_k \ , \qquad (2) \\ \text{subject to} \quad & y_k(\boldsymbol{w}^T\phi(\boldsymbol{x}_k) + b) \geq 1 - \xi_k, \\ & \xi_k \geq 0, k = 1, \ldots, m, \end{aligned}$$

where training data are mapped to a higher dimensional space by the function ϕ, and C is a penalty parameter on the training error. For any testing instance $\boldsymbol{x}$, the decision function (predictor) is

$$f(\boldsymbol{x}) = \operatorname{sgn}\left(\boldsymbol{w}^T\phi(\boldsymbol{x}) + b\right) .$$

Practically, we need only $k(\boldsymbol{x}, \boldsymbol{x}') = \phi(\boldsymbol{x})^T\phi(\boldsymbol{x}')$, the kernel function, to train the SVM. The RBF kernel is used in our experiments:

$$k(\boldsymbol{x}, \boldsymbol{x}') = \exp(-\gamma\|\boldsymbol{x} - \boldsymbol{x}'\|^2) \ . \qquad (3)$$

With the RBF kernel (3), there are two parameters to be determined in the SVM model: C and γ. To get good generalization ability, we conduct a validation process to decide parameters. The procedure is as the following:

1. Consider a grid space of (C, γ) with $\log_2 C \in \{-5, -3, \ldots, 15\}$ and $\log_2 \gamma \in \{-15, -13, \ldots, 3\}$.
2. For each hyperparameter pair (C, γ) in the search space, conduct 5-fold cross validation on the training set.
3. Choose the parameter (C, γ) that leads to the lowest CV balanced error rate.
4. Use the best parameter to create a model as the predictor.

3 Feature Selection Strategies

In this Section, we discuss feature selection strategies tried during the competition. We name each method to be like "A + B," where A is a filter to select features and B is a classifier or a wrapper. If a method is "A + B + C," then there are two filters A and B.

3.1 No Selection: Direct Use of SVM

The first strategy is to directly use SVM without feature selection. Thus, the procedure in Section 2 is considered.

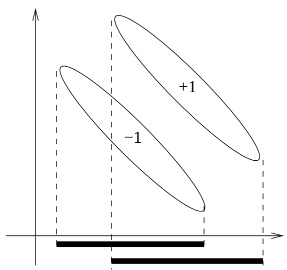
3.2 F-score for Feature Selection: F-score + SVM

F-score is a simple technique which measures the discrimination of two sets of real numbers. Given training vectors $\boldsymbol{x}_k, k = 1, \ldots, m$, if the number of positive and negative instances are n_+ and n_-, respectively, then the F-score of the ith feature is defined as:

$$F(i) \equiv \frac{\left(\bar{\boldsymbol{x}}_i^{(+)} - \bar{\boldsymbol{x}}_i\right)^2 + \left(\bar{\boldsymbol{x}}_i^{(-)} - \bar{\boldsymbol{x}}_i\right)^2}{\frac{1}{n_+-1}\sum\limits_{k=1}^{n_+}\left(x_{k,i}^{(+)} - \bar{\boldsymbol{x}}_i^{(+)}\right)^2 + \frac{1}{n_--1}\sum\limits_{k=1}^{n_-}\left(x_{k,i}^{(-)} - \bar{\boldsymbol{x}}_i^{(-)}\right)^2}, \tag{4}$$

where $\bar{\boldsymbol{x}}_i$, $\bar{\boldsymbol{x}}_i^{(+)}$, $\bar{\boldsymbol{x}}_i^{(-)}$ are the average of the ith feature of the whole, positive, and negative data sets, respectively; $x_{k,i}^{(+)}$ is the ith feature of the kth positive instance, and $x_{k,i}^{(-)}$ is the ith feature of the kth negative instance. The numerator indicates the discrimination between the positive and negative sets, and the denominator indicates the one within each of the two sets. The larger the F-score is, the more likely this feature is more discriminative. Therefore, we use this score as a feature selection criterion.

A disadvantage of F-score is that is does not reveal mutual information among features. Consider one simple example:



Both features of this data have low F-scores as in (4) the denominator (the sum of variances of the positive and negative sets) is much larger than the numerator.

Despite this disadvantage, F-score is simple and generally quite effective. We select features with high F-scores and then apply SVM for training/prediction. The procedure is summarized below:

1. Calculate F-score of every feature.
2. Pick some possible thresholds by human eye to cut low and high F-scores.
3. For each threshold, do the following
   a) Drop features with F-score below this threshold.
   b) Randomly split the training data into X_{train} and X_{valid}.
   c) Let X_{train} be the new training data. Use the SVM procedure in Section 2 to obtain a predictor; use the predictor to predict X_{valid}.
   d) Repeat the steps above five times, and then calculate the average validation error.
4. Choose the threshold with the lowest average validation error.
5. Drop features with F-score below the selected threshold. Then apply the SVM procedure in Section 2.

In the above procedure, possible thresholds are identified by human eye. For data sets in this competition, there is a quite clear gap between high and lower scores (see Figure 1, which will be described in Section 4). We can automate this step by, for example, gradually adding high-F-score features, until the validation accuracy decreases.

3.3 F-score and Random Forest for Feature Selection: F-score + RF + SVM

Random forest (RF) is a classification method, but it also provides feature importance (Breiman 2001). Its basic idea is as follows: A forest contains many decision trees, each of which is constructed by instances with randomly sampled features. The prediction is by a majority vote of decision trees. To obtain feature importance, first we split the training sets to two parts. By training the first and predicting the second we obtain an accuracy value. For the jth feature, we randomly permute its values in the second set and obtain another accuracy. The difference between the two numbers can indicate the importance of the jth feature.

In practice, the RF code we used cannot handle too many features. Thus, before using RF to select features, we obtain a subset of features using F-score selection first. This approach is thus called "F-score + RF + SVM" and is summarized below:

1. F-score
   a) Consider the subset of features obtained in Section 3.2.
2. RF
   a) Initialize the RF working data set to include all training instances with the subset of features selected from Step 1. Use RF to obtain the rank of features.

b) Use RF as a predictor and conduct 5-fold CV on the working set.
c) Update the working set by removing half features which are less important and go to Step 2b.
Stop if the number of features is small.
d) Among various feature subsets chosen above, select one with the lowest CV error.

3. SVM
   a) Apply the SVM procedure in Section 2 on the training data with the selected features.

Note that the rank of features is obtained at Step 2a and is not updated throughout iterations. An earlier study on using RF for feature selection is (Svetnik et al. 2004).

3.4 Random Forest and RM-bound SVM for Feature Selection: RF + RM-SVM

Chapelle et al. (2002) directly use SVM to conduct feature selection. They consider the RBF kernel with feature-wise scaling factors:

$$k(\boldsymbol{x}, \boldsymbol{x}') = \exp\left(-\sum_{i=1}^{n} \gamma_i (x_i - x_i')^2\right) . \tag{5}$$

By minimizing an estimation of generalization errors which is a function of $\gamma_1, \ldots, \gamma_n$, we can have feature importance. Leave-one-out (loo) errors are such an estimation and are bounded by a smoother function (Vapnik 1998):

$$\text{loo} \leq 4\|\tilde{\boldsymbol{w}}\|^2 \tilde{R}^2 . \tag{6}$$

We refer to this upper bound as the radius margin (RM) bound. Here, $\tilde{\boldsymbol{w}}^T \equiv [\, \boldsymbol{w}^T \; \sqrt{C}\boldsymbol{\xi}^T \,]$ and $(\boldsymbol{w}, \boldsymbol{\xi})$ is the optimal solution of the L2-SVM:

$$\min_{\boldsymbol{w}, b, \boldsymbol{\xi}} \frac{1}{2}\boldsymbol{w}^T\boldsymbol{w} + \frac{C}{2}\sum_{k=1}^{m} \xi_k^2 ,$$

under the same constraints of (2); $\tilde{R}$ is the radius of the smallest sphere containing all $[\, \phi(\boldsymbol{x}_k)^T \; \boldsymbol{e}_k^T/\sqrt{C} \,], k = 1, \ldots, m$, where $\boldsymbol{e}_k$ is a zero vector except the kth component is one.

We minimize the bound $4\|\tilde{\boldsymbol{w}}\|^2\tilde{R}^2$ with respect to C and $\gamma_1, \ldots, \gamma_n$ via a gradient-based method. Using these parameters, an SVM model can be built for future prediction. Therefore we call this machine an RM-bound SVM. When the number of features is large, minimizing the RM bound is time consuming. Thus, we apply this technique only on the problem MADELON, which has 500 features. To further reduce the computational burden, we use RF to pre-select important features. Thus, this method is referred to as "RF + RM-SVM."

4 Experimental Results

In the experiment, we use LIBSVM[1] (Chang and Lin 2001) for SVM classification. For feature selection methods, we use the randomForest (Liaw and Wiener 2002) package[2] in software R for RF and modify the implementation in (Chung et al. 2003) for the RM-bound SVM[3]. Before doing experiments, data sets are scaled. With training, validation, and testing data together, we scale each feature to $[0, 1]$. Except scaling, there is no other data preprocessing.

In the development period, only labels of training sets are known. An online judge returns BER of what competitors predict about validation sets, but labels of validation sets and even information of testing sets are kept unknown.

We mainly focus on three feature selection strategies discussed in Sections 3.1-3.3: SVM, F-score + SVM, and F-score + RF + SVM. For RF + RM-SVM, due to the large number of features, we only apply it on MADELON. The RF procedure in Section 3.3 selects 16 features, and then RM-SVM is used. In all experiments we focused on getting the smallest BER.

For the strategy F-score + RF + SVM, after the initial selection by F-score, we found that RF retains all features. That is, by comparing cross-validation BER using different subsets of features, the one with all features is the best. Hence, F+RF+SVM is in fact the same as F+SVM for all the five data sets. Since our validation accuracy of DOROTHEA is not as good as that by some participants, we consider a heuristic by submitting results via the top 100, 200, and 300 features from RF. The BERs of the validation set are 0.1431, 0.1251, and 0.1498, respectively. Therefore, we consider "F-score + RF top 200 + SVM" for DOROTHEA.

Table 1 presents the BER on validation data sets by different feature selection strategies. It shows that no method is the best on all data sets.

Table 1. Comparison of different methods during the development period: BERs of validation sets (in percentage); bold-faced entries correspond to approaches used to generate our final submission

Dataset	ARCENE	DEXTER	DOROTHEA	GISETTE	MADELON
SVM	13.31	11.67	33.98	2.10	40.17
F+SVM	**21.43**	**8.00**	21.38	**1.80**	13.00
F+RF+SVM	21.43	8.00	**12.51**	1.80	13.00
RF+RM-SVM[4]	–	–	–	–	**7.50**

[1] http://www.csie.ntu.edu.tw/~cjlin

[2] http://www.r-project.org/

[3] http://www.csie.ntu.edu.tw/~cjlin/libsvmtools/

[4] Our implementation of RF+RM-SVM is applicable to only MADELON, which has a smaller number of features.

In Table 2 we list the CV BER on the training set. Results of the first three problems are quite different from those in Table 1. Due to the small training sets or other reasons, CV does not accurately indicate the future performance.

Table 2. CV BER on the training set (in percentage)

Dataset	ARCENE	DEXTER	DOROTHEA	GISETTE	MADELON
SVM	11.04	8.33	39.38	2.08	39.85
F+SVM	9.25	4.00	14.21	1.37	11.60

In Table 3, the first row indicates the threshold of F-score. The second row is the number of selected features which is compared to the total number of features in the third row. Figure 1 presents the curve of F-scores against features.

Table 3. F-score threshold and the number of features selected in F+SVM

Dataset	ARCENE	DEXTER	DOROTHEA	GISETTE	MADELON
F-score threshold	0.1	0.015	0.05	0.01	0.005
#features selected	661	209	445	913	13
#total features	10000	20000	100000	5000	500

5 Competition Results

For each data set, we submit the final result using the method that leads to the best validation accuracy in Table 1. A comparison of competition results (ours and winning entries) is in Tables 4 and 5.

Table 4. NIPS 2003 challenge results on December 1st

Dec. 1st	Our best challenge entry					The winning challenge entry					
Dataset	Score	BER	AUC	Feat	Probe	Score	BER	AUC	Feat	Probe	Test
OVERALL	52.00	9.31	90.69	24.9	12.0	88.00	6.84	97.22	80.3	47.8	0.4
ARCENE	74.55	15.27	84.73	100.0	30.0	98.18	13.30	93.48	100.0	30.0	0
DEXTER	0.00	6.50	93.50	1.0	10.5	96.36	3.90	99.01	1.5	12.9	1
DOROTHEA	-3.64	16.82	83.18	0.5	2.7	98.18	8.54	95.92	100.0	50.0	1
GISETTE	98.18	1.37	98.63	18.3	0.0	98.18	1.37	98.63	18.3	0.0	0
MADELON	90.91	6.61	93.39	4.8	16.7	100.00	7.17	96.95	1.6	0.0	0

For the December 1st submissions, we rank 1st on GISETTE, 3rd on MADELON, and 5th on ARCENE. Overall we rank 3rd as a group and our best entry

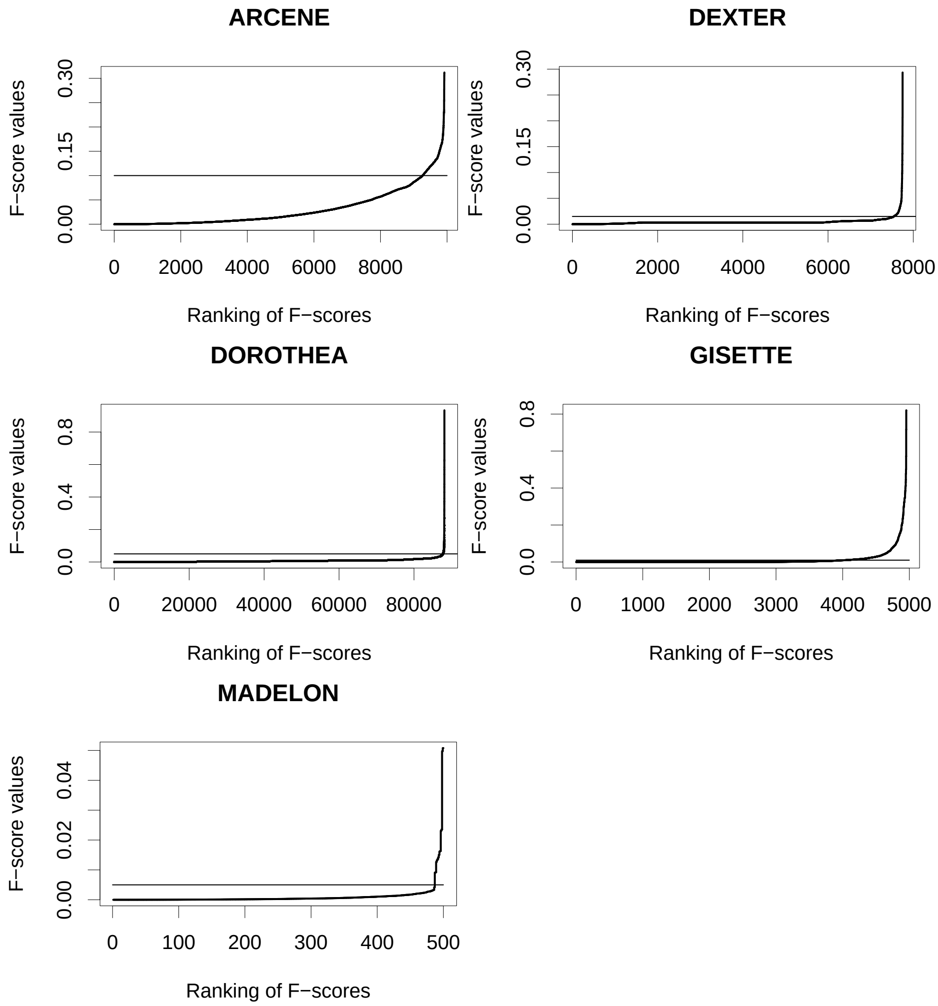


Fig. 1. Curves of F-scores against features; features with F-scores below the horizontal line are dropped

Table 5. NIPS 2003 challenge results on December 8th

Dec. 8th	Our best challenge entry					The winning challenge entry					
Dataset	Score	BER	AUC	Feat	Probe	Score	BER	AUC	Feat	Probe	Test
OVERALL	49.14	7.91	91.45	24.9	9.9	88.00	6.84	97.22	80.3	47.8	0.4
ARCENE	68.57	10.73	90.63	100.0	30.0	94.29	11.86	95.47	10.7	1.0	0
DEXTER	22.86	5.35	96.86	1.2	2.9	100.00	3.30	96.70	18.6	42.1	1
DOROTHEA	8.57	15.61	77.56	0.2	0.0	97.14	8.61	95.92	100.0	50.0	1
GISETTE	97.14	1.35	98.71	18.3	0.0	97.14	1.35	98.71	18.3	0.0	0
MADELON	71.43	7.11	92.89	3.2	0.0	94.29	7.11	96.95	1.6	0.0	1

is the 6^{th}, using the criterion of the organizers. For the December 8^{th} submissions, we rank 2^{nd} as a group and our best entry is the 4^{th}.

6 Discussion and Conclusions

Usually SVM suffers from a large number of features, but we find that a direct use of SVM works well on GISETTE and ARCENE. After the competition, we realize that GISETTE comes from an OCR problem MNIST (LeCun et al. 1998), which contains 784 features of gray-level values. Thus, all features are of the same type and tend to be equally important. Our earlier experience indicates that for such problems, SVM can handle a rather large set of features. As the 5,000 features of GISETTE are a combination of the original 784 features, SVM may still work under the same explanation. For ARCENE, we need further investigation to know why direct SVM performs well.

For the data set MADELON, the winner uses a kind of Bayesian SVM (Chu et al. 2003). It is similar to RM-SVM by minimizing a function of feature-wise scaling factors. The main difference is that RM-SVM uses an loo bound, but Bayesian SVM derives a Bayesian evidence function. For this problem Tables 4- 5 indicate that the two approaches achieve very similar BER. This result seems to indicate a strong relation between the two methods. Though they are derived from different aspects, it is worth investigating the possible connection.

In conclusion, we have tried several feature selection strategies in this competition. Most of them are independent of the classifier used. This work is a preliminary study that for an SVM package what feature selection strategies should be included. In the future, we would like to have a systematic comparison on more data sets.

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