Semi-Supervised Least-Squares Support Vector Classifier based on Virtual Leave One Out Residuals

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Abstract. We present a new semi-supervised learning system based on least-squares support vector machine classifier. We apply the virtual leave-one-out residuals as criterion for selection of the most influential data for label switching test. The analytic form of the solution enables to obtain a high gain of the computational cost. The quality of the method was tested on the artificial data set – two moons problem and on the real signal-averaged ECG data set. The correct classification score is better as compared to other methods.

1 Introduction

The semi-supervised learning consists of numerous methods [1, 2] that attempt to improve the supervised classifier trained on the labelled data subset L by exploring the information contained in the (usually larger) subset of unlabelled input data U. The supervised classifier is considered as an initial hypothesis for classification decisions. In the following steps each unlabelled point is assigned with two alternative labels, +1 or -1, and the decision is made according to the improvement of the quality function. Hence, the computation tasks increase quickly for larger number of unlabelled points [10, 11]. The crucial problem for efficient algorithm is to find simple solution for the supervised learning and to define a smart criterion for the selection of the most influential unlabelled points in order to perform the label switching tests.

Our idea of semi-supervised learning system is to use the least-squares support vector machine (LS-SVM) [3, 4] as supervised classifier and to select unlabelled points for label switching upon their ranking with respect to the virtual leave-one-out residuals (VLOO), the influential statistics [5, 6]. The advantage of our idea comes from the algebraic solution of the LS-SVM and the analytic formula for the VLOO residuals [7, 8, 9]. We also use the VLOO residuals for pruning the final form of the classifier. Our method is tested on the artificial data set (two moons problem) and for

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the real-life signal averaged ECG data set. We named our system semi-supervised least-squares support vector machine (SS-LS-SVM).

2 Semi-Supervised Least Squares Support Vector Machine

2.1 General Idea

The idea of semi-supervised least-squares support vector machine is implemented by the following algorithm:

1. Use LS-SVM classifier for labeled data subset L
2. Initial hypothesis: classify the unlabelled data subset U according to the LS-SVM rule
3. Calculate the virtual leave-one-out residuals for all points L∪U
4. Rank all points upon the VLOO score
5. Take NUM points of largest VLOO residuals for label switching
6. Go to 2 until the PRESS statistics reaches the required minimal value

2.2 Least-Squares Support Vector Machine

LS-SVM originates by changing the inequality constraints in the SVM formulation to equality constraints with objective function in the least squares sense [3, 4].
Data set *D* is defined as:

$$D = \{(\mathbf{x}_i, t_i)\} \qquad \mathbf{x}_i \in X \subset R^d, \quad t_i \in \{-1,+1\} \tag{1}$$

The LS-SVM classifier performs the function:

$$f(\mathbf{x}) = \mathbf{w}\phi(\mathbf{x}) + b \tag{2}$$

This function is obtained by solving the following optimization problem:

$$\mathcal{L} = \frac{1}{2} \| \mathbf{w} \|^2 + \gamma \sum_{i=1}^{l} [t_i - \mathbf{w}\phi(\mathbf{x}_i) - b]^2 \tag{3}$$

In the nonlinear case the kernel function is introduced:

$$K(\mathbf{x}, \mathbf{x}') = \phi(\mathbf{x}) \cdot \phi(\mathbf{x}') \tag{4}$$

Hence, the solution can be expressed as the linear combination of kernels weighted by the Lagrange multipliers α_i:

$$f(\mathbf{x}) = \sum_{i=1}^{l} \alpha_i K(\mathbf{x}_i, \mathbf{x}) + b \tag{5}$$

The global minimizer is obtained in LS-SVM by solving the set of linear equations

$$\begin{bmatrix} \mathbf{K} + \gamma^{-1}\mathbf{I} & \mathbf{1} \\ \mathbf{1}^T & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{\alpha} \\ b \end{bmatrix} = \begin{bmatrix} \mathbf{t} \\ 0 \end{bmatrix} \tag{6}$$

In this work the RBF kernel is applied:

$$K(\mathbf{x}, \mathbf{x}') = \exp\{-\eta \parallel \mathbf{x} - \mathbf{x}'\|^2\} \tag{7}$$

Therefore this system is easier to solve as compared to SVM. However the sparseness of the support vectors is lost. In SVM, most of the Lagrangian multipliers α_i are equal 0 while in LS-SVM the Lagrangian multipliers α_i are proportional to the errors e_i

2.3 Virtual Leave-One-Out Cross-Validation

Leave-one-out cross-validation (LOO) provides the basis for very efficient model selection. The drawback of such approach is its computational complexity. Each step of LOO cross validation of an LS-SVM model requires re-computation of linear equation system (thus inversion of large matrix in case of complex problems) which is computational expensive. One can perform leave-one-out cross-validation in closed form without leaving an example out. Let:

$$y_i = f(\mathbf{x}_i) \tag{8}$$

and

$$\mathbf{C} = \begin{bmatrix} \mathbf{K} + \gamma^{-1}\mathbf{I} & \mathbf{1} \\ \mathbf{1}^T & 0 \end{bmatrix} \tag{9}$$

It can be shown that the virtual residual [7, 8]:

$$r_i^{(-1)} = y_i - y_i^{(-i)} = \frac{\alpha_i}{C_{ii}^{-1}} \tag{10}$$

Hence, the residual r_i can be computed using information already available as a by-product of training the LS-SVM classifier on the whole data set.

3 The Algorithm of the Semi-supervised LS-SVM

The input to the SS-LS-SVM algorithm consists of:

- the data set $data_L$ (which contains labelled data),
- the set L of labels corresponding to the members of the $data_L$ set,
- the data set $data_U$ (which contains unlabelled data),
- integer NUM – the parameter describing how many data points are taken into account during label switching,

- γ, σ - the hyperparameters of the ls-svm model.

We also make use of two external procedures: trainlssvm (which calculates the α and b values of the LS-SVM model) and simlssvm (used for classification).

The output of the algorithm consists of the calculated α and b values of the LS-SVM model, which can be used for classification task.

The algorithm of SS-LS-SVM

```
Require: data_L – labelled samples
data_U – unlabelled samples
L – labels set by the operator,
NUM – parameter of transduction algorithm – number of switched
labels
□,□□- hyperparameters of the lssvm model
trainlssvm – procedure for calculation □ and b parameters of
the model,
simlssvm – classification procedure, returns the labels

Initialization {
  acquire labeled data set L
  //creation of the model based on the labeled data
  [alpha,b]=trainlssvm(data_L, L, RBF kernel, □, □);
  //initial labeling of all data samples
  L'=simlssvm({data_L,L,RBF kernel, □, □},{alpha,b},data_U);
  }
Main loop {
  [alpha,b]=trainlssvm(data_L∪U, L', RBF kernel, □, □);
  for i=1 to N_L∪U compute r_i=alpha_i/C^-1_ii
  //label switching
  for NUM largest r_i {
    switch the label in set L'
    }
  [alpha',b']=trainlssvm(data_L+U, L', RBF kernel, □, □);
  for i=1 to sizeof(data_L∪U) compute r_i=alpha_i/C^-1_ii
  for NUM largest r_i {
    if (r_i'>r_i) set previous label
    }
  }
call pruning procedure
return [alpha, b] //variables describing obtained
                    classifier
```

The algorithm is divided into three stages – a) initialization b) computation stage.and c) pruning stage. During the initialization stage, the ss-ls-svm classifier is trained using the labeled data set $data_L$ only (Fig 1.). Thereafter unlabelled data set $data_U$ is classified according to the LS-SVM rule. The results of classification are stored in the label set L'. This is the initial hypothesis – all previously unlabelled data points are now labeled, however it is possible that not all labels are correct (Fig 2.).

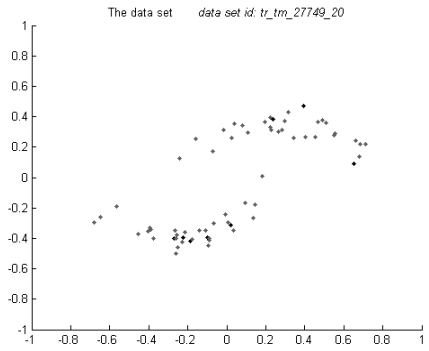


Fig. 1. The initialization stage the SS-LS-SVM classifier – it is trained using the labeled data only (black points).

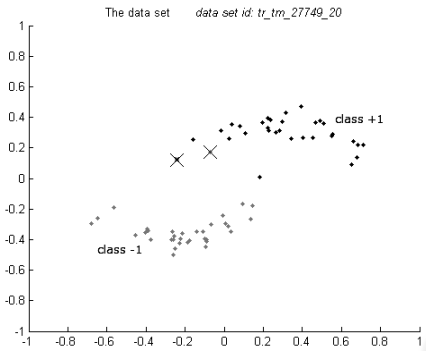


Fig. 2. Initial labelling – marked points represent potentially misclassified data. (black points – class +1, grey – class -1)

In the next stage of the algorithm we try to improve the results of initial labelling. Potentially misclassified data points are selected using the values of virtual residuals r_i (computed using the Virtual Leave-One-Out Cross-Validation method [6]). The labels of the NUM points having largest r_i value are switched to the opposite value. If the r_i value after switching increases then the old label is restored.

Pruning. The last stage of SS-LS-SVM algorithm is pruning of the obtained model by removing the least relevant data points. The original data set and the decision boundary calculated for this data set using the LS-SVM model are shown in Fig. 3. The relevance of the data points is determined by values of virtual residuals r_i (Fig. 4).

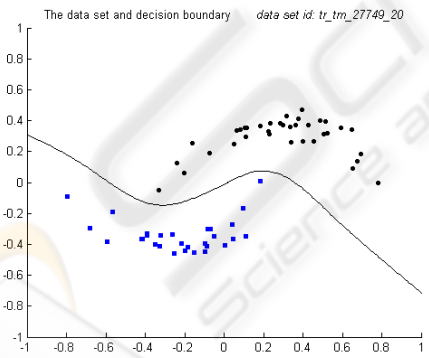


Fig. 3. The decision boundary created using whole learning data set.

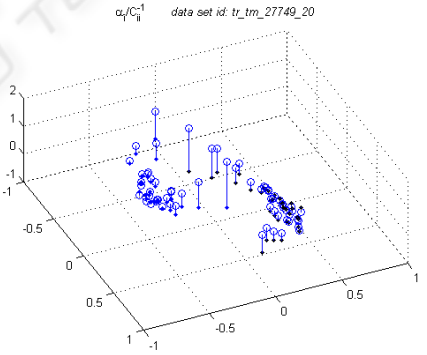


Fig. 4. The values of residuals calculated for all data points.

The pruned data set contains data points which satisfy the rule

$$r_i \geq 0.3 \cdot \max(\{r_i\}) \tag{11}$$

This approach significantly reduces the number of support vectors without loss of the classification score, as shown in Fig. 5.

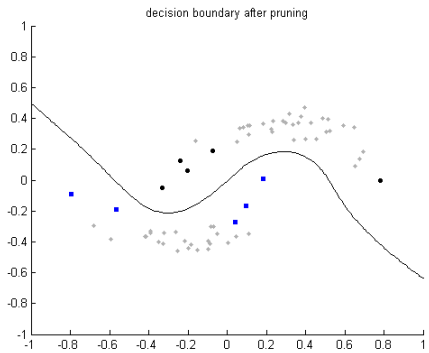


Fig. 5. The result of pruning and the decision boundary after pruning.

4 Evaluation of the SS-LS-SVM on Artificial Data Set

4.1 The Data Sets

The algorithms were evaluated on an artificially generated two dimensional data set "Two moons – tm_27749_20". The data set contains points belonging to two non-linearly separable classes (positive – labelled as +1 and negative – labelled as -1). The set was divided into two subsets – the learning set used for creating of LS-SVM models and the test set for testing of developed algorithms. The training set contains 66 data points: 33 belonging to the positive class and 33 to the negative class (shown in Fig. 3). The test set contains 134 examples: 67 belonging to the positive class and 67 to the negative class.

The second data set tm_94326 was generated by the same algorithm as tm_27749_20. It consists of 2000 data points: 666 points assigned to the learning set and 1334 points of the test set. The data set was used to test the pruning algorithm.

4.2 Evaluation of VLOO Estimator

We studied the properties of VLOO estimator on the "Two moons – tm_27749_20" dataset described in 4.1. We calculated the leave one out error and its virtual counterpart (10) for every data point in the learning set. The diagram shown in Fig. 6 contains the plot of VLOO error versus LOO error. The correlation coefficient is equal 0.95. Therefore we can conclude that VLOO calculated by (10) is sufficiently good estimator of LOO error.

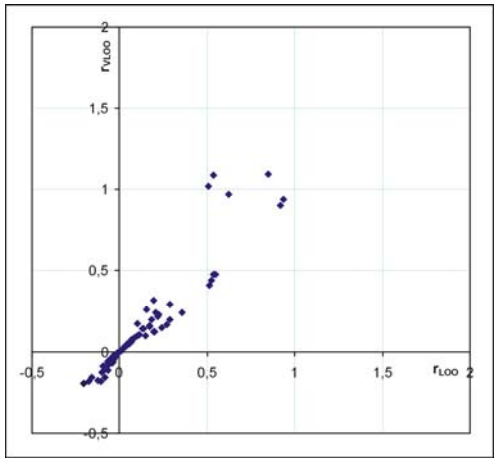
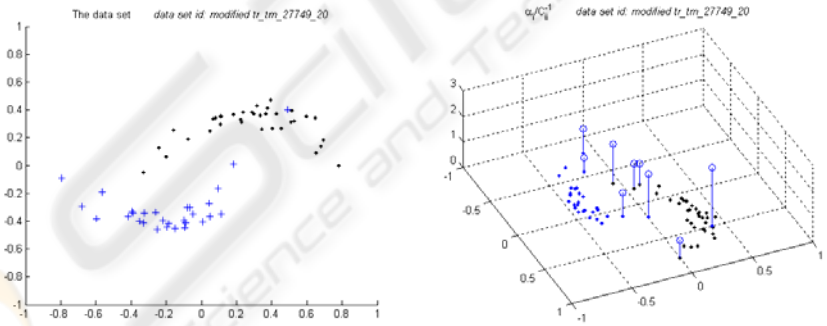


Fig. 6. VLOO versus LOO error.

4.3 Criterion for Finding of Potentially Misclassified Examples

We can use (10) to detect potentially misclassified examples. Figure 7a presents artificially generated two-dimensional data set. One point (0.4890, 0.4002) is intentionally mislabelled. We trained the LS-SVM classifier for the presented data set and performed VLOO procedure calculating the r_i for all points. Figure 7b shows the data samples and the largest corresponding r_i values. As one can see the most influential data samples and our misclassified sample correspond to the largest r_i values.



a) b)

Fig. 7. a) The data set with one point (0.4890, 0.4002) intentionally mislabelled; b) the data set and largest α_i/C_{ii} values – a potential hint for finding misclassified points.

4.4 Results on Artificial Data Set

The tests were performed on the data set tm_27749 described in 4.1. 14 permutations were generated by randomly assigning the points to the test subset and the training

set. Each learning set includes 66 points: 8 points are labeled, 58 points are unlabelled. For the same data the supervised LS-SVM classifier was created. Average error rate of SS-LS-SVM classification results on test set 2.3%. This is twice lower than the error rate calculated for the LS-SVM classifier based on 8 points that is equal 5.6%. The results prove that SS-LS-SVM classifier is independent of the selection of data points to the learning set.

4.5 Pruning Procedure for Two Moons Problem

We tested the pruning procedure on two data sets tm_27749_20 and tm_94326. Applications of pruning procedure to the learning set tm_27749_20 yields in the supervised LS-SVM model that consists of 10 points (the original set comprised 66 points) shown in Fig. 5. The test set classification (using pruned model) yielded in 100% correctly classified examples.

Table 1. Results of pruning procedure applied to 10 permutations of tm_94326 data sets.

	original classifier						**pruned classifier**						
data set	**tp**	**tn**	**fp**	**fn**	**prec**	**recall**	**tp**	**tn**	**fp**	**fn**	**prec**	**recall**	**Model size**
01	673	653	5	3	99,26	99,56	673	653	5	3	99,26	99,56	83
02	657	667	4	6	99,39	99,10	658	671	0	5	100,00	99,25	56
03	661	664	4	5	99,40	99,25	662	664	4	4	99,40	99,40	70
04	646	677	3	8	99,54	98,78	648	678	2	6	99,69	99,08	61
05	665	661	5	3	99,25	99,55	667	663	3	1	99,55	99,85	63
06	654	668	8	4	98,79	99,39	654	668	8	4	98,79	99,39	82
07	668	654	7	5	98,96	99,26	669	653	8	4	98,82	99,41	76
08	648	674	8	4	98,78	99,39	647	674	8	5	98,78	99,23	76
09	661	659	6	8	99,10	98,80	662	659	6	7	99,10	98,95	64
10	657	663	8	6	98,80	99,10	658	663	8	5	98,80	99,25	72
Average					**99,13**	**99,28**					**99,18**	**99,34**	**69**

10 permutations of the tm_94326 data set were generated by randomly assigning the points to the test subset and the training set. For every permutation the supervised LS-SVM classifier was created using the learning set. Such model is based on 666 data points. The performance of the classifiers was checked on the corresponding test data sets (see precision and recall values in Table 1). After application of the pruning procedure the obtained LS-SVM model was evaluated (results are shown in Table 1) on the corresponding test sets.

The average model after pruning comprises 69 data points (versus 666 in the original classifier before pruning procedure). The recall and precision values obtained from the tests of the pruned classifier are similar to the values obtained for the original classifier. The pruning procedure can be safely applied for obtaining of much smaller model with the same excellent properties as its original counterpart.

5 Medical application of SS-LS-SVM

Our study is based on the data set performed at the Warsaw University of Medicine. It consists of 376 patients underwent the signal-averaged ECG recordings [12]. Upon the medical diagnosis, these patients are divided into 3 groups: 100 patients with sustained ventricular tachycardia after myocardial infarction (sVT+), 199 patients without sustained ventricular tachycardia after myocardial infarction (sVT–) and 77 healthy persons.

The signal-averaged ECG signals were recorded using a system with a sampling frequency of 1 kHz. Standard bipolar X,Y,Z leads were used. The time domain analysis of the signal-averaged ECG was performed using FIR filter with the Kaiser window (45-150Hz) [12, 13]. For the filtered signal we calculated 9 parameters [13, 14].

Table 2 contains the results of SS-LS-SVM application to medical dataset. It contains the classification results of the same dataset obtained by 3 different methods: transductive support vector machine (TSVM), transductive least-squares support vector machine (TLS-SVM) based on the Lagrange coefficients ranking and supervised SVM. The score of correct classification for SS-LS-SVM classifier based on only 5% labelled data points is 88.4% - it indicates the advantage of VLOO criterion vs. the Lagrange multiplier ranking. Also, this score is not much worse than that obtained by SVM classifier for the full set of labelled data [14].

Table 2. Classification results of medical data (SVT+).

Method	Labelled data	Correct classifications
SS-LS-SVM (VLOO)	**5%**	**88,4%**
TLS-SVM (based on α)	5%	83,5%
TSVM [14]	50%	94,15%
SVM [14]	100%	95,21%

6 Conclusions

We present the novel approach to semi-supervised learning. The basic idea is the use of information on influential statistics of each labelled point of the data – the leave-one-out residual.

The virtual leave-one–out method (VLOO) enables to obtain the estimated values of leave-one-out score for the entire training set in one step – no retraining is required.

For the semi-supervised least-squares support vector machine all calculations can be expressed in an analytic form.

We applied our approach to the computer-aided medical diagnosis: the recognition of sustained ventricular tachycardia after myocardial infarction. The score of successful recognition (**88.4** % based on **5** % of labelled cases) is meaningful.

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