MINING VERY LARGE DATASETS WITH SVM AND VISUALIZATION

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Keywords: Mining very large datasets, Support vector machines, Active learning, Interval data analysis, Visual data mining, Information visualization.

Abstract: We present a new support vector machine (SVM) algorithm and graphical methods for mining very large datasets. We develop the active selection of training data points that can significantly reduce the training set in the SVM classification. We summarize the massive datasets into interval data. We adapt the RBF kernel used by the SVM algorithm to deal with this interval data. We only keep the data points corresponding to support vectors and the representative data points of non-support vectors. Thus the SVM algorithm uses this subset to construct the non-linear model. We also use interactive graphical methods for trying to explain the SVM results. The graphical representation of IF-THEN rules extracted from the SVM models can be easily interpreted by humans. The user deeply understands the SVM models’ behavior towards data. The numerical test results are obtained on real and artificial datasets.

1 INTRODUCTION

The SVM algorithms proposed by (Vapnik, 1995) are a well-known class of data mining algorithms using the idea of kernel substitution. SVM and kernel related methods have shown to build accurate models. They have shown practical relevance for classification, regression or novelty detection. Successful applications of SVM have been reported for various fields, for example in face identification, text categorization, bioinformatics (Guyon, 1999). SVM and kernel methodology have become increasingly popular data mining tools. Although the prominent properties of SVM, they are not favourable to deal with the challenge of large datasets. SVM solutions are obtained from quadratic programs (QP) possessing a global solution, so that, the computational cost of an SVM approach is at least square of the number of training data points and the memory requirement makes SVM impractical. The effective heuristics to scale up SVM learning task are to divide the original QP into series of small problems (Boser et al., 1992), (Osuna et al., 1997), (Platt, 1999), incremental learning (Syed et al., 1999), (Fung and Mangasarian, 2002) updating solutions in growing training set, parallel and distributed learning (Poulet and Do, 2004) on personal computer (PC) network or choosing interested data points subset (active set) for learning (Tong and Koller, 2000).

While SVM gives good results, the interpretation of these results is not so easy. The support vectors found by the algorithms provide limited information. Most of the time, the user only obtains information regarding the support vectors being used as “black box” to classify the data with a good accuracy. It is impossible to explain or even understand why a model constructed by SVM performs a better prediction than many other algorithms. Therefore, it is necessary to improve the comprehensibility of SVM models. Very few papers have been published about methods trying to explain SVM results (Caragea et al., 2001), (Poulet, 2004).

Our investigation aims at scaling up SVM algorithms to mine very large datasets and using graphical tools to interpret the SVM results.

We develop the active learning algorithm that can significantly reduce the training set in the SVM
classification. Large datasets are aggregated into smaller datasets using interval data concept (one kind of symbolic data (Bock and Diday, 1999)). We adapt the RBF kernel used by the SVM algorithm to deal with these interval data. We only keep the data points corresponding to support interval vectors and the representative data points of non support interval vectors. Thus the SVM algorithm uses this subset to construct the non-linear model. Our algorithm can deal with one million data points in minutes on one personal computer.

We also use interactive graphical methods for trying to explain the SVM results. The interactive decision tree algorithms (Ankerst et al., 1999), (Poulet, 2002) involve the user in the construction of decision tree models on prediction results obtained at the SVM output. The SVM performance in classification task is deeply understood in the way of the IF-THEN rules extracted intuitively from the graphical representation of the decision trees that can be easily interpreted by humans. The comprehensibility of SVM models is significantly improved.

This paper is organized as follows. In section 2, we briefly present SVM algorithm. Section 3 describes our active SVM algorithm that is used to deal with very large datasets. In section 4, we present the inductive rule extraction method for interpreting the SVM result. We demonstrate numerical test results in section 5 before the conclusion and future works in section 6.

2 SVM ALGORITHM

Let us consider a binary linear classification task, as depicted in figure 1, with m data points \( x_1, x_2, \ldots, x_m \) in a n-dimensional input having corresponding labels \( y_i = \pm 1 \).

SVM algorithm aims to find the best separating plane (represented by the vector \( w \) and the scalar \( b \)) as being furthest from both classes. It can simultaneously maximize the margin between the support planes for each class and minimize the error. This can also be accomplished through the quadratic program (1):

\[
\text{Min} \ (1/2) ||w||^2 + C \sum_{i=1}^{m} z_i \\
\text{s.t.} \ y_i (w.x_i - b) + z_i \geq 1 \quad (1)
\]

where the slack variable \( z_i \geq 0 \) (i=1,...,m) and \( C \) is a positive constant used to tune the margin and the error.

![Figure 1: Linear binary classification with SVM](image)

The dual Lagrangian of the quadratic program (1) is:

\[
\text{Min} \ (1/2) \sum_{i=1}^{m} \sum_{j=1}^{m} y_i y_j \alpha_i \alpha_j x_i.x_j - \sum_{i=1}^{m} \alpha_i \\
\text{s.t.} \ \sum_{i=1}^{m} y_i \alpha_i = 0 \quad (2)
\]

\[ C \geq \alpha_i \geq 0 \ (i = 1,\ldots,m) \]

From the \( \alpha_i \) obtained by the solution of (2), we can recover the plane:

\[ w = \sum_{i=1}^{\#SV} y_i \alpha_i x_i \] and the scalar \( b \) determined by the support vectors (for which \( \alpha_i > 0 \)).

And then, the classification function of a new data point \( x \) based on the plane is: \( \text{sign} \ (w.x - b) \)
To change from a linear to nonlinear classification, no algorithmic changes are required from the linear case other than substitution of a kernel evaluation for the simple dot product of (2). And then, it can be tuned into a general nonlinear algorithm:

\[
\text{Min } \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} y_i y_j K(x_i, x_j) - \sum_{i=1}^{m} \alpha_i
\]

s.t. \[\sum_{i=1}^{m} y_i \alpha_i = 0\] (3)

\[C \geq \alpha_i \geq 0 \text{ (i = 1, \ldots, m)}\]

By changing the kernel function \(K\) as a polynomial or a radial basis function, or a sigmoid neural network, we can get different nonlinear classification. The classification of a new data point \(x\) is based on:

\[
\text{sign} \left( \sum_{i=1}^{\#SV} y_i \alpha_i K(x, x_i) - b \right)
\] (4)

SVM algorithms solve the QP (3) being well known at least square of the number of training data points and the memory requirement is expensive. The practical implement methods including chunking, decomposition (Boser et al., 1992), (Osuna et al., 1997) and sequence minimal optimization (Platt, 1999) divide the original QP into series of small problems.

Incremental proximal SVM proposed by (Fung and Mangasarian, 2002) is another SVM formulation very fast to train because it requires only the solution of a linear system. This algorithm only loads one subset of the data at any one time and updates the model in incoming training subsets. The authors have performed the linear classification of one billion data points in 10-dimensional input space into two classes in less than 2 hours and 26 minutes on a Pentium II.

Some parallel and distributed incremental SVM algorithms (Poulet and Do, 2004) or boosting of SVM (Do and Poulet, 2004a) can deal with at least one billion data points on PCs in some minutes.

Active learning algorithms (Tong and Koller, 2000) only use data points closest to the separating plane.

These algorithms can deal with either very large datasets in linear classification problem or non linear classification on medium datasets (in tens of thousands data points).

3 ACTIVE SVM FOR LARGE DATASETS

![Figure 2: SVM learning on active subset](image)

Our active SVM algorithm exploits the separating boundary structure which only depends on training data points closed (support vectors) to it, thick points as depicted in figure 2. The natural clusters of these training data points also relate to the decision boundary of SVM. Therefore, our algorithm selects the clusters closed to the separating boundary. We summarize large datasets into clusters. The SVM algorithm is trained on clusters, we obtain the support vectors at the output containing data points for creating the separating boundary. However, we
need to adapt SVM on high level data clusters. If the clusters are represented by their centers, we can lose information. So that, we use the interval data concept to represent the clusters. A interval vector corresponds to a cluster, the low and high values of an interval are computed by low and high bound of data points in this cluster. After that, we construct non-linear kernel function RBF for dealing with interval datasets.

3.1 Active selection for SVM using interval data concept

\[ K(x, y) = \exp\left(\frac{-2\|x - y\|^2}{\sigma^2}\right) \]  

(5)

Assume we have two data points \( x \) and \( y \in \mathbb{R}^n \), the RBF kernel formula in (5) of two data vectors \( x \) and \( y \) of continuous type is based on the Euclidean distance between these vectors, \( d_{\text{E}}(x, y) = \|x - y\| \).

For dealing with interval data, we only need to measure the distance between two vectors of interval type, after that we substitute this distance measure for the Euclidean distance into RBF kernel formula. Thus the new RBF kernel can deal with interval data. The popular known dissimilarity measure between two data vectors of interval type (Kreinovich et al., 2004) is the Hausdorff distance.

Suppose that we have two intervals represented by low and high values: \( I_1 = [\text{lo}w_1, \text{hi}gh_1] \) and \( I_2 = [\text{lo}w_2, \text{hi}gh_2] \), the Hausdorff distance between two intervals \( I_1 \) and \( I_2 \) is defined by formula (6):

\[ d_{\text{H}}(I_1, I_2) = \max\{|\text{lo}w_1 - \text{lo}w_2|, |\text{hi}gh_1 - \text{hi}gh_2|\} \]  

(6)

Let us consider two data vectors \( u, v \in \Omega \) having \( n \) dimensions of interval type:

\[ u = ([u_{1,\text{low}}, u_{1,\text{high}}], [u_{2,\text{low}}, u_{2,\text{high}}], \ldots, [u_{n,\text{low}}, u_{n,\text{high}}]) \],

\[ v = ([v_{1,\text{low}}, v_{1,\text{high}}], [v_{2,\text{low}}, v_{2,\text{high}}], \ldots, [v_{n,\text{low}}, v_{n,\text{high}}]). \]

The Hausdorff distance between two vectors \( u \) and \( v \) is defined by formula (7):

\[ d_{\text{H}}(u, v) = \sqrt{\sum_{i=1}^{n} \max\{|u_{i,\text{low}} - v_{i,\text{low}}|, |u_{i,\text{high}} - v_{i,\text{high}}|\}^2} \]  

(7)

By substituting the Hausdorff distance measure \( d_{\text{H}} \) into RBF kernel formula, we obtain a new RBF kernel for dealing with interval data. This modification tremendously changes SVM algorithms for mining interval data. No algorithmic changes are required from the habitual case of continuous data other than the modification of the RBF kernel evaluation. All the benefits of the original SVM methods are maintained. We can use SVM algorithms to build interval data mining models in classification, regression and novelty detection. We only focus on the classification problem.

3.2 Algorithm description

We obtain the support interval vectors from learning task on high level representative clusters. We create the active learning subset by extracting data points from the support interval vectors and getting some representative data points of non-support interval vectors. This active subset is used to construct the SVM model. The active learning algorithm is described in table 1. The large dataset is drastically reduced. The algorithm with RBF kernel can classify one million data points in an acceptable execution time (11 hours for creating the clusters and selecting the active learning and 17.69 seconds for constructing the SVM model) on one PC (Pentium-4, 2.4 GHz, 512 MB RAM).
Input: dataset $S = \{\text{positive data points (P), negative data points (N)}\}$

Output: a classification function $f$

Training:

1. Summarize dataset $S$ into interval data $IS = \{\text{interval positive data points, interval negative data points}\}$ using clustering algorithms, 

2. Select support interval vectors (SIV) using SVM algorithm with non-linear RBF kernel function constructed in interval data:

$$SIV = SVM_{train}(IS)$$

3. Active learning dataset $AS$ created by getting representative data points of non-support interval vectors and extracting data points from support interval vectors $SIV$.

4. Construct SVM model with the RBF kernel function on active learning dataset $AS$:

$$f = SVM_{train}(AS)$$

Table 1: Active SVM algorithm

4 INTERPRET SVM RESULTS

Although SVM algorithms have shown to build accurate models, their results are very difficult to understand. Most of the time, the user only obtains information regarding the support vectors being used as “black box” to classify the data with a good accuracy. The user does not know how SVM models can work. For many data mining applications, understanding the model obtained by the algorithm is as important as the accuracy, it is necessary that the user has confidence in the knowledge discovered (model) by data mining algorithms. (Caragea et al., 2001) proposed to use Grand Tour method (Asimov, 1985) to try to visualize support vectors. The user can see the separating boundary between two classes. (Poulet, 2004), (Do and Poulet, 2004b) have combined some strengths of different visualization methods to visualize the SVM results. These methods can detect and show interesting dimensions in the obtained model.

We propose here to use interactive decision tree algorithms, PBC (Ankerst et al., 1999) or CIAD (Poulet, 2002) to try to explain the SVM results. The SVM performance in classification task is deeply understood in the way of IF-THEN rules extracted intuitively from the graphical representation of the decision trees that can be easily interpreted by humans.

Table 2: Inductive rule extraction from SVM models

| Input: non label dataset $SP$ and a SVM classification function $f$ |
| Output: inductive rule set $IND$-RULE |

Extracting:

1. Classify non label dataset $SP$ using SVM classification function $f$, we obtain label set $L$ assigned to $SP$:

$$(SP, L) = SVM_{classify}(SP, f)$$

2. Interactively constructing decision tree model $DT$ on dataset $\{SP, L\}$ using visual data mining decision tree algorithms, i.e. PBC (Ankerst et al., 1999) or CIAD (Poulet, 2002).

3. User extracts inductive rules $IND$-RULE from graphical representation of decision tree model $DT$:

$$IND$-RULE = HumanExtract(graphical $DT$)$$

The rule extraction prototype is described in table 2. We classify dataset using the SVM model, after that the user constructs the decision tree model on the obtained result (dataset and classes predicted by the SVM models). Thus he can easily extract inductive rules from graphical representation of the decision tree model. The SVM models are understood in the way of IF-THEN rules that facilitate human interpretation.

We propose to use the visual data mining decision tree algorithms because they involve more intensively the user in the model construction using interactive visualization techniques. This can help the user to improve the comprehensibility of the obtained model, and thus his confidence in the knowledge discovered is increased.

For example, the SVM algorithm using a RBF kernel separates class 1-against-all in the Segment
Dataset (Michie et al., 1994) having 2310 data points in 19 dimensions with 99.56% accuracy. PBC uses bars to visualize the result at the SVM output (cf. figure 4). Each bar represents one independent dimension. Within it, the values of one dimension are sorted and mapped to pixels (colour = class) in line-by-line according to their order. The user interactively chooses the best separating split to construct the decision tree (based on the human pattern recognition capabilities) or with the help of automatic algorithms. The obtained decision tree (cf. figure 5) having 7 rules can explain 99.80% performance of the SVM model. One rule is created for each path from the root to a leaf, each dimension value along a path forms a conjunction and the leaf node holds the class prediction. And thus, the non linear SVM is interpreted in the way of the 7 inductive rules (IF-THEN) that will be easily understood by humans.

Rule 1: IF (hue-mean < -1.9) THEN CLASS = rest (non brickface)

Rule 2: IF ((-1.9 <= hue-mean < 0.0) and (intensity-mean < 3.6)) THEN CLASS = rest

Rule 3: IF ((-1.9 <= hue-mean < 0.0) and (3.6 <= intensity-mean < 20.9) and (exgreen-mean < -11.9) and (exred-mean < -1.1)) THEN CLASS = brickface

Figure 4: Visualization with PBC of the SVM result on the Segment Dataset (1-against-all)

Figure 5: Visualization of the decision tree explaining the SVM result on the Segment Dataset
Rule 4: IF ((-1.9 <= hue-mean < 0.0) and (3.6 <= intensity-mean < 20.9) and (exgreen-mean < -11.9) and (exred-mean >= -1.1)) THEN CLASS = rest

Rule 5: IF ((-1.9 <= hue-mean < 0.0) and (3.6 <= intensity-mean < 20.9) and (exgreen-mean >= -11.9)) THEN CLASS = brick face

Rule 6: IF ((-1.9 <= hue-mean < 0.0) and (intensity-mean > = 20.9)) THEN CLASS = rest

Rule 7: IF (hue-mean >= 0.0) THEN CLASS = rest

The user uses these rules for interpreting the performance of the SVM model. This can help him to deeply understand how the SVM algorithm can work.

6 CONCLUSION

We have developed a new active SVM algorithm for mining very large (10^6 data points) datasets on personal computers. The main idea is to choose the active training data points that can significantly reduce the training set in the SVM classification. We summarize the massive datasets into interval data. We adapt the RBF kernel used by the SVM algorithm to deal with this interval data. We only keep the data points corresponding to support vectors and the representative data points of non support vectors. Thus the SVM algorithm uses this subset to construct the non-linear model with good results.

We also propose to use interactive decision tree algorithms for trying to explain the SVM results. The user can interpret the SVM performance in classification task in the way of IF-THEN rules extracted intuitively from the graphical representation of the decision trees that can be easily interpreted by humans.

The first future work will be to use high level representative data for searching the SVM parameters. This approach drastically reduces the cost compared with the research in initial large datasets.

Another one will be to extend our approach combining visualization methods and automatic

5 NUMERICAL TEST RESULTS

To evaluate the performance of our active SVM algorithm on very large datasets, we have added to the publicly available toolkit, LibSVM (Chang and Lin, 2003) a new code of the RBF kernel for dealing with interval data. Thus, the software program is able to deal with both interval and continuous data in classification. We focus on numerical tests with large datasets (cf. table 3) generated by the RingNorm program from (Delve, 1996). It is a 20 dimensional, 2 class classification example. Each class is drawn from a multivariate normal distribution. Class 1 has mean zero and covariance 4 times the identity. Class 2 has mean (m, m, ..., m) and unit covariance with m = 2/sqrt(20). We use one Pentium-4, 2.4 GHz, 512 MB RAM running Linux Redhat 9.0 for all experiments. The large datasets are aggregated into smaller ones (interval data) using the K-means algorithm (MacQueen, 1967).

The results obtained by SVM with the RBF kernel function in table 3 show that our active SVM algorithm chooses efficiently the active learning sets in large datasets for training SVM models. Therefore, the learning time and memory requirement are drastically reduced. Thus the algorithm is able to deal with non linear classification in massive datasets (10^6 data points) on one personal computer in acceptable execution time.

<table>
<thead>
<tr>
<th>Table 3: Classification results on large datasets</th>
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<tbody>
<tr>
<td>Dataset 1</td>
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<tr>
<td>Training set:</td>
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<tr>
<td>Testing set:</td>
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<tr>
<td>Interval data</td>
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<tr>
<td>Clustering time</td>
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<td>Active set</td>
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<td>Learning time</td>
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<td>Support vectors</td>
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<td>Accuracy</td>
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The user uses the rules for interpreting the performance of the SVM model. This can help him to deeply understand how the SVM algorithm can work.
algorithms for mining very large datasets and interpreting the results too.

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