epsilon-Support Vector and Large-Scale Data Mining Problems*

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Abstract. Data mining and knowledge discovery has made great progress during the last fifteen years. As one of the major tasks of data mining, classification has wide business and scientific applications. Among a variety of proposed methods, mathematical programming based approaches have been proven to be excellent in terms of classification accuracy, robustness, and efficiency. However, there are several difficult issues. Two of these issues are of particular interest of this research. The first issue is that it is challenging to find optimal solution for large-scale dataset in mathematical programming problems due to the computational complexity. The second issue is that many mathematical programming problems require specialized codes or programs such as CPLEX or LINGO. The objective of this study is to propose solutions for these two problems. This paper proposed and applied mathematical programming model to classification problems to address two aspects of data mining algorithm: speed and scalability.

Keywords: Data mining, Classification, Mathematical Programming, Multiple criteria decision making, Support Vector Machine.

1 Introduction

Over the years, optimization-based algorithms have shown their effectiveness in data mining classification (e.g., Bugera, Konno, and Uryasev, 2002) and Mathematical programming (MP) based algorithm is one of the optimization-based classification algorithms (e.g., Kou et al 2006). Nevertheless, due to the limitation of computation power and memory, it is difficult to apply the MP algorithm, or similar optimization algorithms, to huge datasets which may contain millions of observations. As the size

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of today's databases is continuously increasing, it is highly important that data mining algorithms are able to perform their functions regardless of the sizes of datasets.

Develop mining algorithms that scale to real-life massive databases is the first research challenges proposed by Bradley, Fayyad, and Mangasarian in their overview of applying mathematical programming for data mining. They also pointed out that "approaches that assume that data can fit in main memory need to be revised or redesigned (Bradley, Fayyad, and Mangasarian 1998)." MP based algorithm is such an approach that requires the data to fit in main memory. This requirement comes from the fact that constraint matrix must be loaded into main memory in order to achieve an acceptable computation time and the size of constraint matrix is determined by the size of the training dataset. Therefore, as the size of dataset increases, the computation time increases and performance degraded.

The objectives of this research are: (1) to propose a new epsilon-support vector approach, and (2) to apply this approach to large scale data mining problem and analyze substantial datasets (size of $O(10^9)$). The results indicate that this new approach has the potential to handle arbitrary-size of datasets.

This paper is organized in three parts. The next section describes the epsilon-support vector for Multi-criteria Convex Quadratic programming (MCQP) two-group classification model. Section 3 presents the experimental results. The last section concludes the paper.

2 Epsilon-Support Vector (eSV) Approach

Each row of a $n \times r$ matrix $A = (A_1, \dots, A_n)^T$ is a vector $A_i = (a_{i1}, \dots, a_{ir}) \in \mathbb{R}^r$ which corresponds to one of the records in the training dataset of a binary classification problem, $i = 1, \dots, n$; n is the total number of records in the dataset. Two groups, G_1 and G_2 , are predefined while $G_1 \cap G_2 = \Phi$ and $A_i \in \{G_1 \cup G_2\}$. A boundary scalar b can be selected to separate G_1 and G_2 . Let $X = (x_1, \dots, x_r)^T \in \mathbb{R}^r$ be a vector of real number to be determined. In the classification problem, $A_i X$ is the score for the i^{th} data record. If all records are linear separable and an element A_i is correctly classified, then let β_i be the distance from A_i to b , and consider the linear system, $A_i X = b - \beta_i$, $\forall A_i \in G_1$ and $A_i X = b + \beta_i$, $\forall A_i \in G_2$. However, if we consider the case where the two groups are not linear separable because of mislabeled records, a "Soft Margin" and slack distance variable α_i need to be introduced. Previous equations now transforms to $A_i X = b + \alpha_i - \beta_i$, $\forall A_i \in G_1$ and $A_i X = b - \alpha_i + \beta_i$, $\forall A_i \in G_2$. To complete the definitions of β_i and α_i , let $\beta_i = 0$ for all misclassified elements and α_i equals to zero for all correctly classified elements. Incorporating the definitions of β_i and α_i , our classification models could be set as:

$$\text{Minimize } \frac{1}{2} \|X\|_2^2 + W_\alpha \sum_{i=1}^n \alpha_i^2 - W_\beta \sum_{i=1}^n \beta_i + \frac{W_b}{2} b^2$$

$$\text{Subject to: } Y(\langle A \cdot X \rangle - eb) = \delta' e - \alpha + \beta$$

where Y is a given $n \times n$ diagonal matrix, $e = (1, 1, \dots, 1)^T$, $\alpha = (\alpha_1, \dots, \alpha_n)^T$, $\beta = (\beta_1, \dots, \beta_n)^T$, X and b are unrestricted.

The Lagrange function corresponding to Model 3 is

$$L(X, b, \eta, \theta) = \frac{1}{2} \|X\|_2^2 + \frac{W_\alpha}{2} \sum_{i=1}^n \eta_i^2 + W_\beta \sum_{i=1}^n \eta_i + \frac{W_b}{2} b^2 - \theta^T (Y(\langle A \cdot X \rangle - eb) - e\delta' + \eta)$$

where $\theta = (\theta_1, \dots, \theta_n)^T$, $\eta = (\eta_1, \dots, \eta_n)^T$, $\theta_i, \eta_i \in \Re$.

$$\begin{aligned} \text{According to Wolfe Dual Theorem, } \nabla_X L(X, b, \eta, \theta) &= X - A^T Y \theta = 0, \\ \nabla_b L(X, b, \eta, \theta) &= W_b b + e^T Y \theta = 0, \quad \nabla_\eta L(X, b, \eta, \theta) = W_\alpha \eta + W_\beta e - \theta = 0. \end{aligned} \quad (3)$$

Introduce the above 3 equations to the constraints of Model 3, we can get:

$$\begin{aligned} Y((A \cdot A^T)Y\theta + \frac{1}{W_b} e(e^T Y\theta)) + \frac{1}{W_\alpha} (\theta - W_\beta e) &= \delta' e \\ \Rightarrow \theta &= \frac{(\delta' + \frac{W_\beta}{W_\alpha})e}{\frac{I}{W_\alpha} + Y((A \cdot A^T) + \frac{1}{W_b} ee^T)Y} \end{aligned} \quad (4)$$

In algorithm, we describe how to use this model in a classification problem.

Algorithm

Input: a $n \times r$ matrix A as the training dataset, a $n \times n$ diagonal matrix Y labels the class of each record.

Output: classification accuracies for each group in the training dataset, score for every record, decision function $((X^* \cdot A_i) - b^*) \begin{cases} > 0, \Rightarrow A_i \in G_1 \\ \leq 0, \Rightarrow A_i \in G_2 \end{cases}$

Step 1. compute $\theta^* = (\theta_1, \dots, \theta_n)^T$ by (5). W_β, W_α, W_b are chosen by cross validation.

Step 2. compute $X^* = A^T Y \theta^*$, $b^* = \frac{-1}{W_b} e^T Y \theta^*$.

Step 3. classify a incoming A_i by using decision function $((X^* \cdot A_i) - b^*) \begin{cases} > 0, \Rightarrow A_i \in G_1 \\ \leq 0, \Rightarrow A_i \in G_2 \end{cases}$.

END

In existing SVM approaches (Boser et al 1992), the sparsity of the optimal α_i^* (many of $\alpha_i^* = 0$) is the key in solving large scale SVM problem and the support vectors ($\alpha_i^* = 0$) are the points at the hyperplane. Similarly, the support vector A_i of our models can be defined as $\alpha_i^* = \beta_i^* = 0$. Due to the formulation of the model objectives, almost none of the data points A_i lie on two adjusted bounding hyperplanes $b \pm 1$. Thus most of the time α_i^* and β_i^* do not equal to zero simultaneously. A Karush-Kuhn-Tucker (KKT) condition that has been used in previous support vector approaches (Cristianini and Shawe-Taylor 2000, Schölkopf, and Smola 2002) can not be held any more because of the introduction of distance variable β_i in our model. As a result, we need to establish another condition for those data points A_i whose corresponding $|\alpha_i^* - \beta_i^*| < \mathcal{E}$ to define the epsilon-support vectors (eSVs) such that the computation complexity can be reduced for large scale problems. $\mathcal{E}$ is picked so that only a small part (e.g. 1%) of the records belongs to epsilon-support vectors. Generally, if $n < 1000000$, Model 2 can use the whole dataset; otherwise, a sample training set (e.g. 1% of the population) can be randomly generated from the original data. Using the sample set, we can find an optimal solution and epsilon-support vectors for the original dataset. All epsilon-support vectors are used to re-train the model repeatedly until the classification results meet certain criteria/threshold. A stratified random sampling approach is incorporated into our algorithm for large scale data mining problem ($>O(10^9)$).

Stratified Random Sampling

Since MP based algorithm requires training datasets to fit in main memory, the size of training dataset is limited by the capacity of main memory ($O(10^{6-8})$). One possible solution is to use only part of the training dataset when the dataset size is extremely huge ($>O(10^9)$). However, this approach may loss valuable information that exists in the unused part of the training dataset. In order to make the best use of the training dataset, we employ a revised stratified random sampling.

Let's briefly describe how standard stratified random sampling works. First, the dataset is partitioned into groups of data called strata. Each data belongs to one and only one stratum. Second, a sample is selected by some design within each stratum (Thompson 1992). As a sampling technique, the goal of stratified random sampling is to select a portion of a population that can be used as a "representation" of the population as a whole.

Algorithm

The following procedure summarized the whole process:

Algorithm 1

Input: The training dataset A as the population, n is the number of observation in the population and is a huge number; m is the number of

subpopulations which can be fitted into main memory; The testing dataset A'; Algorithm Stop criteria.

Output: Average classification accuracies; decision scores for all observations; decision function.

Step 1: A is evenly partitioned into m subpopulations or strata by random selection.

Step 2: One random sample is drawn from each of m subpopulations and formulate the first training set Tr.

Step 3: Compute $\theta^* = (\theta_1, \dots, \theta_n)^T$ using Tr as input. W_β, W_α, W_b are chosen by cross validation.

Step 4: Compute $X^* = A^T Y \theta^*$, $b^* = \frac{-1}{W_b} e^T Y \theta^*$. If the performance measure meet pre-set criteria (accuracy, total computation time, etc) and the iteration times > 10 , stop; otherwise go to step 5.

Step 5: Compute $|\alpha_i^* - \beta_i^*|$ for all observations in A.

Step 6: Suppose we have n_1 observations (epsilon-support vectors (eSVs)) corresponding $|\alpha_i^* - \beta_i^*| < \varepsilon$ and n_2 observations (Non epsilon-support vectors) which $|\alpha_i^* - \beta_i^*| > \varepsilon$. Formulate a new set with all n_1 eSVs and some ($n_3, n_3 \leq n_2$ and $n_3 \cong 10\% * n_1$) non eSVs. If $(n_3 + n_1) \leq m$, the new set is the new training set, otherwise, random sample m observations from the new set to formulate a train set. Go back to step 3.

END

* Iteration times must be greater than 10 to minimize the influence of the selection of initial training dataset.

3 Experimental Results

The purpose of this research is to test the applicability of our algorithm in large scale data mining problem ($> O(10^9)$), which is too large to be loaded into a typical PC memory (512MB-4Gb) but can be saved in harddisk (40Gb-1Tb). Because we can't find any real life data in such size, we use a Normally Distributed Clustered program (NDC) (Musicant 1998) to generate datasets. Normally distributed cluster is a data generator. NDC generates data points clustered to a series of random centers and all points are multivariate normal distributed. All variables are integers for simplicity. Then, NDC randomly generates a separating plane and assign a class for each random center according to the random separating plane. NDC changes dataset separability by changing the variances of the distributions. The percentage of separability is calculated by counting how many points end up on the right and wrong side of the separating plane. NDC will provide the percentage of linear separability.

The experimental study has two parts. The first one is to test the capability of the proposed algorithm in massive problem with low noises. The second test is to evaluate the performance of the proposed algorithm under high noises, large dataset.

Massive Dataset

The first experiment dataset consists of 100 million records and each record has 20 variables. It is balanced with 50% of the data in the first group and 50% of the data in the second group. The dataset is 95% linear separable (Musicant 1998).

Algorithm 2

Input: The input data set of 100 million records; Assume that at most 1 million records can be fitted into main memory.

Output: 10-fold cross validation average classification accuracies; computing time.

Step 1: The input data set is evenly partitioned into 10 subsets by stratified random sampling selection.

Step 2: A standard 10-fold cross-validation set of 10 sets of training dataset and testing dataset is stored by using one of the 10 subsets as the testing dataset and using the remaining 9 subsets as training dataset. Repeat the following steps for each of the 10 sets of training dataset and testing dataset

Step 3: $n=100$ million and $m=1$ million. Stop criteria: Prediction Accuracy > 94.8% or computing time > 1000 minutes. Apply algorithm 1.

END

Table 1. Massive dataset computing results

10-fold	training		time	testing	
	Class 1	Class 2	(seconds)	Class 1	Class 2
fold 1	94.93%	94.87%	631	94.91%	94.82%
fold 2	94.96%	94.82%	933	94.93%	94.82%
fold 3	94.85%	94.93%	378	94.87%	94.91%
fold 4	94.88%	94.89%	785	94.87%	94.90%
fold 5	94.84%	94.95%	655	94.82%	94.93%
fold 6	94.95%	94.93%	1217	94.89%	94.91%
fold 7	94.93%	94.93%	467	94.91%	94.86%
fold 8	94.98%	94.85%	632	94.92%	94.84%
fold 9	94.87%	94.94%	876	94.85%	94.83%
fold 10	94.83%	94.88%	539	94.84%	94.86%
average	94.90%	94.90%	711.3	94.88%	94.87%

Large Dataset with High Noise

The first experiment dataset consists of 2 million records and each record has 10 variables. It is balanced with 50% of the data in the first group and 50% of the data in the second group. The dataset is 75% linear separable.

Algorithm 3

Input: The input data set of 2 million records; Assume that all records can be fitted into main memory.

Output: 10-fold cross validation average classification accuracies; computing time.

Step 1: The input data set is evenly partitioned into 10 subsets by stratified random sampling selection.

Step 2: A standard 10-fold cross-validation set of 10 sets of training dataset and testing dataset is stored by using one of the 10 subsets as the testing dataset and using the remaining 9 subsets as training dataset. Repeat the following steps for each of the 10 sets of training dataset and testing dataset

Step 3: $n=2$ million and $m=2$ million. Stop criteria: Prediction Accuracy > 70% or computing time > 1000 minutes. Apply algorithm 1.

END

Table 2. High noise dataset computing results

10-fold	training		time	testing	
	Class 1	Class 2	(seconds)	Class 1	Class 2
fold 1	71.34%	74.33%	1279	70.25%	71.12%
fold 2	72.77%	74.13%	849	72.85%	72.47%
fold 3	74.79%	72.44%	1537	72.31%	71.23%
fold 4	70.94%	73.58%	2574	70.32%	72.09%
fold 5	74.11%	72.35%	742	72.57%	71.32%
fold 6	73.56%	74.33%	1380	73.24%	72.67%
fold 7	71.90%	70.38%	3546	70.39%	70.12%
fold 8	73.89%	72.48%	836	72.37%	72.23%
fold 9	72.37%	73.38%	711	71.56%	71.73%
fold 10	73.56%	72.84%	1207	72.40%	72.19%
average	72.92%	73.02%	1466.1	71.83%	71.72%

4 Conclusion

In this research, we proposed a new epsilon-support vector approach and conducted 2 experimental studies using computer generated large scale classification problem to address two aspects of data mining algorithm: speed and scalability. The experimental results indicate that the new approach is capable in solving large scale data mining problems ($>O(10^9)$) and highly efficient (computing time complexity $O(n^{1.5-2})$). This approach also has good performance when the dataset is highly noisy (noises are larger than 25% of the whole data).

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