Efficient Algorithm for Linear Pattern Separation

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Abstract. We propose cutting plane algorithm for solving the linear pattern separation problem, which is a particular case of the more general topic of data mining. The solution we provided, based on convex programming, can also be applied to any other pattern separation scheme based on a convex discriminant like *linear piecewise* or *quadratic* models. Some experimentations are reported with different large databases together with a comparison with a direct implementation with two commercial specialized codes.

1 Introduction

Linear separation [1,5] is an important concept in data mining [3,6]. It is widely used and has been applied in many fields, e.g., *cancer diagnosis*, *human genome*, *game strategies*, *pattern recognition*, *decision/selection making*, and others. Many other separation rules can be found in the litterature, and our method can handle those of them that are based on a functional rule expressed by a convex form. In some cases the size of the data set [2] is so large that solving the mathematical programming problem becomes a challenge even with the state-of-the-art optimization software. In this paper we propose to resort a so-called cutting plane method to solve the problem efficiently, and we discuss ways to improve performance on the linear separation problem.

2 Problem Formulation

Given a set of points $\mathcal{A} = \{a_i \in \mathcal{R}^n, i = 1, 2, \dots, N\}$, and a partition $\mathcal{S}_1 \cup \mathcal{S}_2$ of the set of indices $\mathcal{S} = \{1, 2, \dots, N\}$, we wish to find $w \in \mathcal{R}^n$ and $\gamma \in \mathcal{R}$ such that the hyperplane $\{x \mid w^T x = \gamma\}$ separates the two subsets $\mathcal{A}(\mathcal{S}_1)$ and $\mathcal{A}(\mathcal{S}_2)$, where

$$\mathcal{A}(\mathcal{S}_1) = \{a_i \in \mathcal{A} \mid i \in \mathcal{S}_1\}, \quad (1)$$

$$\mathcal{A}(\mathcal{S}_2) = \{a_i \in \mathcal{A} \mid i \in \mathcal{S}_2\}. \quad (2)$$

For typographical convenience, we will write (w, γ) instead of (w^T, γ) .

Actually, one looks for a strong separation. Thus, given a *separation margin* $\nu > 0$, we hope to achieve the separation properties (3-4) displayed bellow

$$\forall a_i \in \mathcal{A}(\mathcal{S}_1) \quad w^T a_i \geq \gamma + \nu, \quad (3)$$

$$\forall a_i \in \mathcal{A}(\mathcal{S}_2) \quad w^T a_i \leq \gamma - \nu. \quad (4)$$

In general, there is no guarantee that the two sets can be strongly separated. Therefore, for any choice of w and γ , we might observe *misclassification errors*, which we define as follows

$$e_i^1 = \frac{\max(-w^T a_i + \gamma + \nu, 0)}{\|(w, \gamma, \nu)\|}, \quad i \in \mathcal{S}_1, \quad (5)$$

$$e_i^2 = \frac{\max(w^T a_i - \gamma + \nu, 0)}{\|(w, \gamma, \nu)\|}, \quad i \in \mathcal{S}_2. \quad (6)$$

Our goal is then to build a separation hyperplane $\{x \mid w^T x = \gamma\}$ (i.e., compute w and γ) for which the total sum of *misclassification errors* is minimal. In other words, we want to find a vector w and a scalar γ such that the average sum of misclassifications errors is minimized [5].

The separation margin ν helps avoiding the useless trivial solution $(w, \gamma) = (0, 0)$. Its value is usually set to 1. In some cases the separation margin may lead to large values for w and γ . It may be necessary [2] to bound w to avoid this undesirable feature; so, we add the constraint $\|w\|_2 \leq k$.

Formally, we have to solve the following optimization problem

$$\min_{(w, \gamma) \in \mathcal{R}^n \times \mathcal{R}} \left[\frac{1}{|\mathcal{S}_1|} \sum_{i \in \mathcal{S}_1} \max(-w^T a_i + \gamma + \nu, 0) + \frac{1}{|\mathcal{S}_2|} \sum_{i \in \mathcal{S}_2} \max(w^T a_i - \gamma + \nu, 0) \right] \quad (7)$$

$$\text{subject to: } \|w\|_2 \leq k. \quad (8)$$

In ACCPM the square normed in the constraint $\|w\|^2 \leq k^2$ is also treated as black box. If $\bar{w}$ is not feasible ($\|\bar{w}\|^2 > k^2$), the constraint

$$w + 2\langle \bar{w}, w - \bar{w} \rangle \leq k^2 \quad (9)$$

holds for any feasible point.

Finally, let us give two bounds on f . Since $f(0, 0) = 2\nu$, then 2ν is an upper bound of the optimal value of the objective. A straightforward lower bound is 0, but this can be only attained if perfect classification is achieved.

Let us discuss now the formulation of problem (7)–(8) as a standard mathematical programming problem. Let z_i , $i \in \mathcal{S}$, be an auxiliary variable. The original problem becomes

$$\min_{\substack{(w, \gamma) \in \mathcal{R}^n \times \mathcal{R} \\ z \geq 0}} \frac{1}{|\mathcal{S}_1|} \sum_{i \in \mathcal{S}_1} z_i + \frac{1}{|\mathcal{S}_2|} \sum_{i \in \mathcal{S}_2} z_i \quad (10)$$

$$\text{subject to: } z_i \geq (-w^T a_i + \gamma + \nu), \, i \in \mathcal{S}_1 \tag{11}$$

$$z_i \geq (w^T a_i - \gamma + \nu), \, i \in \mathcal{S}_2 \tag{12}$$

$$\|w\|_2 \leq k. \tag{13}$$

Note that the constraints (11)–(12) are numerous but linear. The problem is thus a large linear programming problem with one quadratic constraint (13). Some authors [2] prefer to replace the quadratic constraint by a quadratic penalty term in the objective. Another possibility consists in replacing the Euclidean norm in (13) by the ℓ_∞ norm [4]. The problem becomes then fully linear.

Table 1. Comparison with direct methods

n	m	MOSEK(1)	CPLEX(1)	MOSEK(2)	CPLEX(2)	ACCPM
10	10000	2.54	1.95	6.31	1.81	1.95
20	10000	2.21	2.47	11.37	2.35	2.63
30	10000	4.45	4.45	18.70	4.12	3.40
40	10000	6.34	6.11	23.78	5.99	4.50
50	10000	9.23	8.18	26.11	8.20	4.95
60	10000	11.84	11.10	30.78	11.10	6.30
70	10000	15.13	13.07	40.87	12.82	8.86
80	10000	19.87	15.00	50.21	14.21	10.16
90	10000	26.04	19.97	69.20	19.46	15.03
100	10000	30.22	22.19	62.63	21.29	16.81
10	100000	143.86	81.08	113.40	78.12	5.11
20	100000	120.47	109.53	132.25	108.29	8.22
30	100000	172.21	143.98	179.24	141.31	10.59
40	100000	253.38	194.34	215.89	190.40	16.31
50	100000	311.35	223.71	280.87	219.60	16.95
60	100000	576.77	273.46	303.09	285.38	18.97
70	100000	742.84	408.01	411.66	396.50	28.88
80	100000	850.15	427.15	478.61	406.19	31.25
90	100000	906.57	496.57	590.95	439.29	34.06
100	100000	1443.25	543.25	680.81	493.78	40.30

(1) simplex

(2) interior point

3 Implementation

In our experiments we have considered various sample data sets to test our algorithm, all generated radonmly using a normal distribution.

The problem were solved using the public release of ACCPM. All our experiments were conducted on a 500 Mhz SUN Ultrasparc with 256 MB of RAM. For problems with a very large data set, we performed an out-of-core computation. With a buffer of 200,000 elements, five accesses to disk per iteration were required.

We compare our method with direct methods based on a standard linear programming (LP) formulation of the problem. Recall that the linear programming formulation was given in (10)–(12). (Note that we drooped the norm constraint (13).) The (dual) LP formulation can be solved using standard techniques of linear programming such as *simplex* or *interior point methods*. We have compared ACCPM with two linear programming codes: MOSEK and CPLEX. Both offer the options between a simplex and a primal-dual log barrier algorithm. Table 1 displays our experimental results.

4 Conclusion

We have proposed a cutting plane algorithm for the linear pattern separation problem. The main idea was to modeling the problem through the purpose of minimizing the total misclassification gap as a convex function. Experimentations and comparative study show that our method is quiet efficient even when consider very large databases.

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