



Convex Hulls in Solving Multiclass Pattern Recognition Problem

D. N. Gainanov^{1,2}, P. F. Chernavin², V. A. Rasskazova^{1(✉)},
and N. P. Chernavin²

¹ Moscow Aviation Institute, Moscow, Russia
damir.gainanov@gmail.com, varvara.rasskazova@mail.ru

² Ural Federal University, Ekaterinburg, Russia
chernavin.p.f@gmail.com

Abstract. The paper proposes an approach to solving multiclass pattern recognition problem in a geometric formulation based on convex hulls and convex separable sets (CS-sets). The advantage of the proposed method is the uniqueness of the resulting solution and the uniqueness of assigning each point of the source space to one of the classes. The approach also allows you to uniquely filter the source data for the outliers in the data. Computational experiments using the developed approach were carried out using academic examples and test data from public libraries.

Keywords: Multiclass pattern recognition · Convex hull · Machine learning algorithm

Introduction

The paper deals with multiclass pattern recognition problem in a geometric formulation. Different approaches to solving such a problem could be found in [1, 2, 5, 8, 12, 15, 18, 19, 21]. Mathematical models for solving applied pattern recognition problems are considered in [1–4, 12, 13]. In this paper there is proposed a method for solving this problem which is based on the idea of separability of convex hulls of sets of training sample. The convex-hulls and other efficient linear approaches for solving similar problems were also proposed in [2, 6, 7, 17]. To implement this method, two auxiliary problems are considered: the problem of selecting extreme points in a finite set of points in the space \mathbb{R}^n , and the problem of determining the distance from a given point to the convex hull of a finite set of points in the space \mathbb{R}^n using tools of known software packages for solving mathematical programming problems. An efficiency and power of the proposed approach are demonstrated on classical Irises Fischer problem [16, 22] as well as on several applied economical problems.

Let a set of n -dimensional vectors be given in the space \mathbb{R}^n

$$A = \{\mathbf{a}_i = (a_{i1}, a_{i2}, \dots, a_{in})\} : i = [1, N], \quad (1)$$

and let there also be given a separation of this set into m classes

$$A = A_1 \dot{\cup} A_2 \dot{\cup} \dots \dot{\cup} A_m. \tag{2}$$

You need to construct a decision rule for assigning an arbitrary vector a_i to one of the m classes.

There are a number of methods [14,23] for solving this multiclass pattern recognition problem in a geometric formulation: linear classifiers, committee constructions, multiclass logistic regression, methods of support vectors, nearest neighbors, and potential functions. These methods are related to metric classification methods and are based on the ability to measure the distance between classified objects, or the distance between objects and hypersurfaces that separate classes in the feature space. This paper develops an approach related to convex hulls of subsets $A_i, i = [1, m]$, of the family A .

1 Multiclass Pattern Recognition Algorithm Based on Convex Hulls

The main idea of the proposed approach is as follows.

Let for the given family of points A , which is separated into m classes A_i where $i \in [1, m]$, corresponding convex hulls $conv A_i$ contain only points from classes A_i respectively. Then it is natural to assume that any point $x \in conv A_i$ represents a vector belonging to the class A_i . Below, we will extend this idea for the general case.

Definition 1. *The set A_i from (2), where $i \in [1, m]$, is named a convex separable set (CS-set, CSS), if the following holds*

$$conv A_i \cap A_j = \emptyset, \forall j \in [1, m] \setminus \{i\}. \tag{3}$$

If the family $A = \{A_1, \dots, A_m\}$ contains a CSS A_{i_0} , then it is natural to assume that each point $x \in conv A_{i_0}$ belongs to the corresponding set A_{i_0} . In such a case the set A_{i_0} can be excluded from the further process of constructing the decision rule. In other words, the condition $x \in conv A_{i_0}$ must be checked first, and further process on the assigning point x to one of classes from training sample, must continue if and only if $x \notin conv A_{i_0}$.

An interesting case of families (1) is when you can specify a sequence (i_1, i_2, \dots, i_m) , which is a permutation for the sequence $(1, 2, \dots, m)$, and such that

$$\begin{cases} conv A_{i_1} \cap \bigcup_{k=2}^m A_{i_k} = \emptyset, \\ conv A_{i_2} \cap \bigcup_{k=3}^m A_{i_k} = \emptyset, \\ \dots, \\ conv A_{i_{m-1}} \cap A_m = \emptyset. \end{cases} \tag{4}$$

The problem of constructing a decision rule for the family (1) with properties (4) will be called as CSS-solvable.

We denote by $class(x)$ the class number of $[1, m]$, to which the point x belongs. Thus, if $x \in A_i, i \in [1, m]$, then $class(x) = i$. For the point $x \notin A$, the problem of pattern recognition in the geometric formulation is to construct a decision rule for determining $class(x)$ for $x \in \mathbb{R}^n \setminus A$.

Let's consider the case of $m = 2$, i.e. $A = A_1 \cup A_2$. Let's construct convex hulls $conv A_1$ and $conv A_2$. It is natural to assume that if $x \in conv A_1 \setminus conv A_2$, then $class(x) = 1$.

Similarly, if $x \in conv A_2 \setminus conv A_1$, then we assume that $class(x) = 2$. If $x \notin conv A_1 \cup conv A_2$, it is natural to assume that the point x belongs to such a class whose convex hull is located closer to the point x .

Let's denote by $\rho(x, conv A')$ the distance from the point x to the convex hull of a finite set $A' \subset \mathbb{R}^n$. Then we have $class(x) = arg \min_{i \in \{1, 2\}} \{\rho(x, conv A_i)\}$.

Finally, let's consider the case of $x \in conv A_1 \cap conv A_2$.

Let's consider the following two sets.

$$\begin{aligned} A'_1 &= A_1 \cap conv A_1 \cap conv A_2, \\ A'_2 &= A_2 \cap conv A_1 \cap conv A_2. \end{aligned} \tag{5}$$

Logically there are possible cases:

$$\left. \begin{aligned} 1. & A'_1 = \emptyset, A'_2 = \emptyset \\ 2. & A'_1 \neq \emptyset, A'_2 = \emptyset \\ 3. & A'_1 = \emptyset, A'_2 \neq \emptyset \\ 4. & A'_1 \neq \emptyset, A'_2 \neq \emptyset \end{aligned} \right\} \tag{*}$$

Following the assumption mentioned above, i.e. $x \in conv A_1 \cap conv A_2$, we have:

$$\begin{aligned} class(x) & \text{ is not defined for the case 1,} \\ class(x) & = 1 \text{ for the case 2,} \\ class(x) & = 2 \text{ for the case 3.} \end{aligned}$$

Case 4 leads us to the following situation.

We have a family of two subsets $A' = \{A'_1, A'_2\}$, which locate inside the set $conv A_1 \cap conv A_2$. You need to construct a decision rule for assigning the vector $x \in conv A_1 \cap conv A_2$ to one of the two classes A'_1, A'_2 and, respectively, A_1, A_2 .

This problem corresponds to the original one, and therefore the proposed algorithm can be re-applied. Repeating the process we become to situation when for regular sets of the form (5) there holds $conv A''_1 \cap conv A''_2 = \emptyset$, and thus the process will be completed.

Proposition 1. *If for the sets A_1, A_2 we have $A_1 \cap A_2 = \emptyset$, then algorithm described above converges, i.e. for any point x from $A_1 \cup A_2$ it will lead to the case 1, 2 or 3 (*).*

Proof. Let's consider the following chain of pairs of sets

$$\begin{aligned}
 A &= A_1 \cup A_2, \quad C_1 = \text{conv } A_1, C_2 = \text{conv } A_2: \\
 A_1^{(1)} &= A_1 \cap C_1 \cap C_2 \\
 A_2^{(1)} &= A_2 \cap C_1 \cap C_2 \\
 A^{(1)} &= A_1^{(1)} \cup A_2^{(1)}, \quad C_1^{(1)} = \text{conv } A_1^{(1)}, C_2^{(1)} = \text{conv } A_2^{(1)} \\
 A_1^{(2)} &= A_1^{(1)} \cap C_1^{(1)} \cap C_2^{(1)} \\
 A_2^{(2)} &= A_2^{(1)} \cap C_1^{(1)} \cap C_2^{(1)} \\
 \dots \\
 A^{(k-1)} &= A_1^{(k-1)} \cup A_2^{(k-1)}, \quad C_1^{(k-1)} = \text{conv } A_1^{(k-1)}, C_2^{(k-1)} = \text{conv } A_2^{(k-1)} \\
 A_1^{(k)} &= A_1^{(k-1)} \cap C_1^{(k-1)} \cap C_2^{(k-1)} \\
 A_2^{(k)} &= A_2^{(k-1)} \cap C_1^{(k-1)} \cap C_2^{(k-1)} \\
 A^{(k)} &= A_1^{(k)} \cup A_2^{(k)}, \quad C_1^{(k)} = \text{conv } A_1^{(k)}, C_2^{(k)} = \text{conv } A_2^{(k)} \\
 \dots
 \end{aligned}$$

Let's show that at some step one of the conditions $A_1^{(k)} = \emptyset$ or $A_2^{(k)} = \emptyset$ will be hold, which means that the proposed algorithm converges.

Let's show that at any step we will have $\left| A_1^{(k+1)} \cup A_2^{(k+1)} \right| < \left| A_1^{(k)} \cup A_2^{(k)} \right|$.

Since $A_1 \cap A_2 = \emptyset$, then $A_1^{(k)} \cap A_2^{(k)} = \emptyset$.

On the other hand,

$$A_1^{(k+1)}, A_2^{(k+1)} \subseteq \text{conv } A_1^{(k)} \cap \text{conv } A_2^{(k)}. \tag{6}$$

Let's show that there is a point $x \in A_1^{(k)} \cup A_2^{(k)}$ such that $x \in \text{conv } A_1^{(k)} \cap \text{conv } A_2^{(k)}$. Let's assume the opposite:

$$\begin{cases}
 A_1^{(k)} \subseteq \text{conv } A_1^{(k)} \cap \text{conv } A_2^{(k)}, \\
 A_2^{(k)} \subseteq \text{conv } A_1^{(k)} \cap \text{conv } A_2^{(k)}.
 \end{cases} \tag{7}$$

Therefore, we have

$$\begin{cases}
 \text{conv } A_1^{(k)} \subseteq \text{conv } A_1^{(k)} \cap \text{conv } A_2^{(k)}, \\
 \text{conv } A_2^{(k)} \subseteq \text{conv } A_1^{(k)} \cap \text{conv } A_2^{(k)}.
 \end{cases} \tag{8}$$

On the other hand, by the definition of a convex hull, we get

$$\begin{cases}
 \text{conv } A_1^{(k)} \supseteq \text{conv } A_1^{(k)} \cap \text{conv } A_2^{(k)}, \\
 \text{conv } A_2^{(k)} \supseteq \text{conv } A_1^{(k)} \cap \text{conv } A_2^{(k)}.
 \end{cases} \tag{9}$$

From (8) and (9) there follows that

$$\text{conv } A_1^{(k)} = \text{conv } A_2^{(k)}. \tag{10}$$

From (10) there follows that

$$\begin{cases}
 \text{ext} \left(\text{conv } A_1^{(k)} \right) = \text{ext} \left(\text{conv } A_2^{(k)} \right) \subseteq A_1^{(k)}, \\
 \text{ext} \left(\text{conv } A_2^{(k)} \right) = \text{ext} \left(\text{conv } A_1^{(k)} \right) \subseteq A_2^{(k)}.
 \end{cases} \tag{11}$$

Hence, $A_1^{(k)} \cap A_2^{(k)} \neq \emptyset$, which contradicts the assumption above. Thus, the proposition is proved.

Let's consider the case $m > 2$.

Just as in the case of $m = 2$, the solution of the multiclass pattern recognition problem is reduced to solving a series of similar problems characterized by a sequential decreasing their dimensions. To characterize such a problem, we need to specify the following.

$$\left. \begin{aligned}
 X' \subset \mathbb{R}^n & \text{ — subset of points for which the problem is solving,} \\
 A' = \{A'_i \subseteq A : i \in J \subseteq [1, m]\} & \text{ — the family of finite sets,} \\
 & \text{for which the problem is solving,} \\
 C(A') = \{C'_i = \text{conv}A'_i : i \in J \subseteq [1, m]\} & \text{ — the family of convex hulls} \\
 & \text{of the sets of the family } A'_i, \\
 J' \subseteq J & \text{ — the set of classes, which take part in the problem.}
 \end{aligned} \right\} \quad (12)$$

Let's denote by $\langle x', X', J', A', C(A') \rangle$ the problem of determining whether a point $x' \in X'$ belongs to one of the classes $J' \subset J$, provided by training sample A' with a set of convex hulls $C(A')$.

Further classification of the point $x' \in X'$ will be determined by the value

$$M' = \left| \left\{ i \in J' : x' \in C'_i \right\} \right|$$

and will break up into 3 cases: $M' = 0$, $M' = 1$ and $M' > 1$. Let rules of obtaining the problem $\langle x'', X'', J'', A'', C(A''), M'' \rangle$ in case $|M'| > 1$ are as following:

$$\left. \begin{aligned}
 x'' &= x', \\
 J'' &= \left\{ i \in J' : x'' \in C'_i \right\}, \\
 M'' &= |J''|, \\
 X'' &= \cap \left\{ C'_i : i \in J'' \right\}, \\
 A'' &= \left\{ A''_i = A'_i \cap X'' : i \in J'' \right\}, \\
 C(A'') &= \left\{ C''_i = \text{conv}A''_i : i \in J'' \right\}.
 \end{aligned} \right\} \quad (13)$$

Thus, the decision rule for a multiclass pattern recognition problem based on convex hulls can be represented as a hierarchical tree of basic problems of the form (12). And the root of this tree is the problem of the form $Z = \langle x, \mathbb{R}^n, J = [1, m], A, C(A) \rangle$.

Let's denote by $Z(J')$ a problem of the form (13), which is obtained from the problem Z for the set $J' \subseteq J$ such that

$$\bigcap \{C_i : i \in J'\} \neq \emptyset. \tag{14}$$

Let $\{J'_1, \dots, J'_{k_1}\}$ be the family of all subsets of $J' \subseteq J$ satisfying (14). Then for the problem Z of the first level, we get k_1 problems of the form $Z(J'_i)$, $i \in [1, k_1]$, of the second level. For each second-level problem of the form $Z(J'_i)$, a series of next-level problems of the form $Z(J'_i)(J''_i)$ will be obtained, and so on. A vertex in such a hierarchical tree becomes terminal if the subsample A involved in its formulation is included in no more than in one convex hulls involved in its formulation. Thus, to construct a decision rule, you need to construct a hierarchical graph of problems of the form (12) by constructing convex hulls for obtaining subsamples located in at least two convex hulls of the generating problem. To implement such an algorithm for constructing a decision rule, it is necessary to have effective algorithms for solving the following problems.

- (1) Let a finite set $A \subseteq \mathbb{R}^n$ be given. You need to find all extreme points of its convex hull $ext(conv A)$.

To detect either a point x is an extreme one for a finite set A , you could to solve a following problem LP1 from [20] (see also [24]).

Let a_j denote an element of A .

$$\min x_j : \sum_{i \in I} x_i a_i = a_j, \sum_{i \in I} x_i = 1, x_i \geq 0 \forall i \in I,$$

where I denotes the set $\{1, 2, \dots, n\}$.

It also should be mentioned that [20] provide an efficient algorithm to solving a problem on the detecting all extreme points of a finite set A by solving a sequence of problems of the form LP1.

- (2) Let a point x and a set $ext(M)$ of extreme points of the polyhedron M be given. You need to determine whether the point x belongs to the polyhedron M , i.e. is it true that $x \in conv ext(M)$?

The LP 2 problem can be used to solve this problem.

Let $x \in \mathbb{R}^n$ and $A = \{a_1, a_2, \dots, a_m\} \subseteq \mathbb{R}^n$, and let you need to determine either a point x will belongs to $conv A$.

Let's consider the following system.

$$\begin{cases} \sum_{i=1}^m \alpha_i a_i = x, \\ \sum_{i=1}^m \alpha_i = 1, \\ \alpha_i \geq 0, i \in [1, m]. \end{cases} \tag{15}$$

It's obvious that $x \in convA$ if and only if a system above is feasible. From the other hand, such a system could be transformed into linear program LP2 of the form:

$$\begin{cases} v + w \rightarrow \min, \\ \sum_{i=1}^m \alpha_i a_i = x, \\ \sum_{i=1}^m \alpha_i + v - w = 1, \\ \alpha_i \geq 0, i \in [1, m], \\ v \geq 0, w \geq 0. \end{cases} \tag{16}$$

where v and w are correcting variables in case a system (15) is infeasible. So, a point x will belong to $convA$ if and only if $g = 0$.

- (3) Let a point b and a set $ext(M)$ of extreme points of the polyhedron M be given.

You need to find the shortest distance from the point x to M , i.e. $\rho(x, M) = \min \{\rho(x, y) : y \in M\}$.

The following quadratic programming problem can be used to solve this problem:

$$\begin{cases} \sum_{i=1}^n (x_i - b_i)^2 \rightarrow \min, \\ \sum_{j=1}^m \alpha_j \cdot a_j = x, \\ \sum_{j=1}^m \alpha_j = 1, \\ \alpha_j = 0, j \in [1, m]. \end{cases} \tag{17}$$

Then we get that the required shortest distance from the point b to the convex hull of a finite set A in the space \mathbb{R}^n is equal to the following:

$$\rho(b, conv A) = \sqrt{\sum_{i=1}^n (x_i - b_i)^2}.$$

2 Application of the CSS Machine Learning Algorithm

Let's consider several applied problems, for which proposed CSS machine learning algorithm could be used. Such problems are the problem on the bank scoring [9], analysis of financial markets [10, 11], medical diagnostics, non-destructive control, and search for reference clients for marketing activities in social networks.

Problem 1. A Classical Problem of Irises Fisher [16]

There is a training sample of 150 objects in the space \mathbb{R}^n , which is divided into 3 classes: class A_1 —Setosa, class A_2 —Versicolor and class A_3 —Virginica, and

each class contains 50 objects. It turns out that this well-known classical problem is CSS-solvable:

$$\begin{cases} conv A_1 \cap (A_2 \cup A_3) = \emptyset, \\ conv A_2 \cap A_3 = \emptyset. \end{cases}$$

In this case, the $class(x)$ decision rule looks as following:

$$class(x) = \begin{cases} 1, & x \in conv A_1, \\ 2, & x \in conv A_2, x \notin conv A_1 \\ 3, & x \in conv A_3, x \notin conv A_1. \end{cases}$$

$$arg \min_{i \in \{1,2,3\}} \rho(x, conv A_i), \quad x \notin conv A_1 \cup conv A_2 \cup conv A_3.$$

Problem 2

The proposed approach was used to develop a strategy for trading shares of the Bank of the Russian Federation^{1,2}. 5 stock market indicators were selected as input parameters. Table 1 below provides a description of these parameters.

Table 1. Description of features

No.	Indicator	Values range
1	How many days with no break a moving average convergence divergence (MACD) becomes > than 0 or < than 0	Integer
2	Slow stochastic oscillator signal (SSO)	From 0 to +1
3	How many days with no break SSO gives a strong signal	Integer
4	Relative strength index signal (RSI),	From 0 to +1
5	How many days with no break RSI gives a signal	Integer

The following object classes were required to be recognized:

1. Class **Yes**—the set of positions on the trading strategy that were closed with a profit and the profit was greater than the maximum loss for the period of holding the position.

¹ When opening a position on the exchange, the position is constantly re-evaluated at current prices. Accordingly, the maximum loss on the position is the maximum amount of reduction in the value of the position relative to the value of the position when opening.

² Position hold period is the time from the moment of initial purchase or sale of a certain amount of financial instrument to the moment of reverse in relation to the first trading operation. For more information about the concept of opening and closing positions, see https://www.metatrader5.com/ru/mobile-trading/android/help/trade/positions_manage/open_positions (accessed 01.09.2019).

2. Class **No**—the set of positions on the trading strategy that were closed with a loss or the profit was less than the maximum loss for the period of holding the position.

Corresponding classes were formed based on real data obtained in the period from 26.02.10 until 03.10.19.

Description of cardinality of obtained sets, as well as the number of extreme points and belonging to convex hulls, are shown in the following Table 2.

Table 2. Description of obtained results

	Level 1	Level 2	Level 3
The set Yes	125	82	51
An extremal Yes	47	38	40
% An extremal	37.60 %	46.34%	78.43%
Yes in the convex hull of the Yes only	43	31	4
% Yes in the convex hull of the Yes	34.40%	37.80%	7.84%
Yes in the convex hull of the No	82	51	47
% Yes in the convex hull of the No	65.60%	62.20%	92.16%
The set No	416	290	179
An extremal No	83	84	68
% An extremal	19.95%	28.97%	37.99%
No in the convex hull of the No only	126	111	167
% No in the convex hull of the No	30.29%	38.28%	93.30%
No in the convex hull of the Yes	290	179	12
% No in the convex hull of the Yes	69.71%	61.72%	6.70%

From the table above you can conclude that a position needs to be open if and only if current status corresponds to the convex hull of the class **Yes** of the Level 1 or 2. And in other cases the risk is very high.

Problem 3

Convex hulls method was used for solving the problems on the bank scoring. Let’s describe the most representative examples of favorable and unfavorable cases we had meet.

Favorable Case. There are 6 input parameters, and all of them are related with financial well-being of the borrower. Data from the first stage of calculations are shown in Table 3.

Further the procedure needs to be repeating for the next 9858 non-default and 242 default items. We will not explain all stages, but it should be mentioned that an acceptable solution was obtained with 7 iterations.

Table 3. Favorable case. First stage

Non-default	15000	Default	300
Including an extreme one	320	Including an extreme one	112
Outside of the Default convex hull	5142	Outside of the Non-default convex hull	58
% Definable in the unique way	34.28	% Definable in the unique way	19.33

Unfavorable Case. There are 5 input parameters (loan amount, loan term, borrower age, loan amount-to-age ratio, loan amount-to-loan term ratio). Data from the first stage of calculations are shown in Table 4.

Table 4. Unfavorable case. First stage

Non-default	62635	Default	1347
Including an extreme ones	612	Including an extreme ones	69
Outside of the Default convex hull	1148	Outside of the Non-default convex hull	29
% Definable in the unique way	1.83	% Definable in the unique way	2.15

In this case, the convex hulls of default and non-default sets are significantly intersected, which is due to the specifics of the problem (the share of default loans is 2.1%), as well as to small number of explanatory features. Further we plan to develop a method for solving similar problems (if one set is fully belongs to the another one and strongly blurred in it). In particular, we plan to consider a problem on the determining the balance between the percentage of points included in the convex hull and the size of this convex hull.

It is naturall that practical situations are much more complicated, but the sequence of actions described above allows you to get an efficient desicion rule.

Conclusion

The paper proposes an approach to solving multiclass pattern recognition problems in geometric formulation based on convex hulls and convex separable sets (CS-sets). Such problems often arise in the field of financial mathematics, for example, in problems of bank scoring and market analysis, as well as in various areas of diagnostics and forecasting. The main idea of the proposed approach is as follows. If for the given family of points A, which is separated into m classes A_i where $i \in [1, m]$, each convex hull $conv A_i$ contains only points from class A_i , then we suppose that any point $x \in conv A_i$ represents a vector belonging to the class A_i . In the paper is introduced key definition of convex separable set (CSS) for the family of $A = \{A_1, \dots, A_m\}$ subsets of \mathbb{R}^n . Based on this definition another important for this approach definition of CSS-solvable family $A = \{A_1, \dots, A_m\}$ is introduced. The advantage of the proposed method is

the uniqueness of the resulting solution and the uniqueness of assigning each point of the source space to one of the classes. The approach also allows you to uniquely filter the source data for the outliers in the data. Computational experiments using the developed approach were carried out using academic examples and test data from public libraries. An efficiency and power of the proposed approach are demonstrated on classical Irises Fischer problem [16] as well as on several applied economical problems. It is shown that classical Irises Fischer problem [16] is CSS-solvable. Such a fact allows you to expect a high efficiency of the proposed method from the applied point of view.

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