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Towards multicriteria clustering: An extension of the *k*-means algorithm

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Abstract

The research within the multicriteria classification field is mainly focused on the assignment of actions to pre-defined classes. Nevertheless the building of multicriteria categories remains a theoretical question still not studied in detail. To tackle this problem, we propose an extension of the well-known *k*-means algorithm to the multicriteria framework. This extension relies on the definition of a multicriteria distance based on the preference structure defined by the decision maker. Thus, two alternatives will be similar if they are preferred, indifferent and incomparable to more or less the same actions. Armed with this multicriteria distance, we will be able to partition the set of alternatives into classes that are meaningful from a multicriteria perspective. Finally, the examples of the country risk problem and the diagnosis of firms will be treated to illustrate the applicability of this method.

Keywords: Multiple criteria analysis; Clustering; Preference modeling; *k*-means algorithm

1. Introduction

In many situations, decision makers have to group alternatives (objects or actions) into homogeneous classes. Several examples can be cited:

- in finance, especially in business failure prediction, credit risk assessment or country risk assessment;
- in marketing, for the analysis of the characteristics of customers to design the market penetration strategies;
- in medical diagnosis, for the classification of patients into diseases groups, on the basis of a set of symptoms.

The two mostly used techniques for grouping objects with similar properties are: classification and clustering. Both are often confused, but some important differences exist between them. Classification techniques use supervised learning; what means that the objects are assigned to pre-defined classes. On the contrary, clustering is an unsupervised technique that finds potential groups in data such that, the objects within a same cluster are more similar to each other than to objects in other clusters. Several approaches such as expert systems, neural networks, mathematical programming,

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multicriteria decision aid (MCDA) [19,20], ..., have been explored to deal with this problem. This paper is focused on the MCDA approach.

In the MCDA methodology, grouping alternatives into homogeneous classes consists in assigning a set of alternatives $A = \{a_1, a_2, \ldots, a_n\}$ evaluated on m criteria $\{g_1, g_2, \ldots, g_m\}$ to one of the categories while examining their intrinsic value. The categories are pre-defined by norms called profiles, which separate them or play the role of central reference objects in these categories. The assignment of an alternative to a specific class results from a comparison of its evaluation on all criteria with the profiles defining the categories.

Among the MCDA methods developed to solve these kinds of problems we can mention: Tricotomic Segmentation [14,17,18], ELECTRE TRI [15,21,25], PROAFTN [3], Filtering methods based on concordance and non discordance [16], the UTADIS method [7,11] based on the criteria aggregation model and the Rough set approach [22]. These procedures can be considered as supervised learning methods. As far as we know, in MCDA literature, there are few unsupervised learning techniques [6]. In this paper we are focused on this problematic: regrouping alternatives into a restricted number of categories which will remain as homogeneous as possible. Recently, Zopounidis and Doumpos [26] made a literature review on MCDA classification and sorting methods. We refer the interested reader to this study.

The k-means algorithm [12] is one of the most widely used unsupervised technique. This method allows to group the alternatives into categories in such a way that the distances between the alternatives, within a same category are the shortest, while the distances between the centers of different categories are the largest. Following the multicriteria approach, we are interested in defining a notion of distance between alternatives that takes into account the multicriteria nature of the problem.

In this paper, we present an extension of the k-means algorithm to the multicriteria framework. The intuition behind the method is the following: all actions within the same cluster are preferred, indifferent and incomparable to more or less the same actions following the decision maker preferences. Let us note that this resembles, in the spirit at least, to the sociometric idea of structural equivalence [24]. To quantify this similarity we introduce a multicriteria distance based on the preference structure (P, I, J) defined by the decision maker. The originality of this approach is the application of this new measure within the well-known k-means framework.

The outline of this paper is as follows. In Section 2, we will introduce some important concepts to develop our MCDA clustering approach. The algorithm itself will be presented in Section 3. Section 4 will be dedicated to the study of two applications: the country risk problem and the diagnosis of firms. Finally we will conclude with some general remarks about the method and directions for future research.

2. MCDA clustering

In this section, we describe our clustering method which is an extension of the well-known k-means algorithm with a MCDA background.

In a highly summarized way, the method starts with k prototypes (centroids) that are randomly chosen among all the actions. The alternatives are then assigned to the cluster represented by the nearest prototype. To determine this assignment we introduce a multicriteria distance based on the preference structure defined by the decision maker. Once this step has been done, the prototypes of each cluster are updated by means of a voting procedure. These few steps are repeated until the cluster membership no longer changes. We obtain then a partition of the set of alternatives into k classes.

In the following subsections, we will focus ourselves on the concepts needed to develop this clustering model.

2.1. Preference modeling

The comparison of alternatives is a central component of any decision problem and is naturally grounded on the consequences and attributes of these alternatives. Furthermore, this comparison process can be led between existing actions or with norms or profiles defining fictitious actions.

In preference modeling we usually consider the following relations: Preference (P), Indifference (I), and Incomparability (J), which result from the comparison between two actions a_i and $a_j \in A$.

$$\begin{cases} a_iPa_j & \text{if } a_i \text{ is preferred to } a_j, \\ a_iIa_j & \text{if } a_i \text{ is indifferent to } a_j, \\ a_iJa_j & \text{if } a_i \text{ is incomparable to } a_j. \end{cases}$$

Indeed, these relations translate situations of preference, indifference and incomparability and it can be assumed that they satisfy the following requirements:

$$\forall a_i, a_j \in A \begin{cases} a_iPa_j \Rightarrow a_j\neg Pa_i & : P \text{ is asymmetric,} \\ a_iIa_i & : I \text{ is reflexive,} \\ a_iIa_j \Rightarrow a_jIa_i & : I \text{ is symmetric,} \\ a_i\neg Ja_i & : J \text{ is irreflexive,} \\ a_iJa_j \Rightarrow a_jJa_i & : J \text{ is symmetric.} \end{cases}$$

Definition 1 [23]. The three relations $\{P, I, J\}$ make up a preference structure on A if they satisfy the above conditions and if, given any two elements a_i, a_j of A, one and only one of the following properties is true: a_iPa_j, a_jPa_i, a_iIa_j, a_iJa_j.

2.2. Profile

Our clustering model is based on the idea that all the actions inside the same cluster are similar in the sense that they are preferred, indifferent and incomparable to more or less the same actions. To determine this potential similarity we introduce the notion of profile to each action.

Let $A = \{a_1, a_2, \ldots, a_n\}$ be a set of elements, called actions and let $G = \{g_1, g_2, \ldots, g_m\}$ be a set of m criteria. The application of classic multicriteria tools (Utility Theory, Outranking methods (Electre, Promethee,...), AHP,...) and the concepts of preference modeling mentioned in the previous subsection lead to define $\langle P, I, J\rangle$ (Preference, Indifference and Incomparability) relations $\forall a_i, a_j \in A$. However, it is important to note that only outranking methods lead to define the incomparability relation J. When applying other methods, AHP or Utility Theory for instance, the J relation will remain empty and the comparison between pairs of actions will be restricted to P and I relations.

Once these relations are elicited, any action can be characterized with respect to $\langle A, P, I, J\rangle$:

Definition 2. The profile $P(a_i)$ of action $a_i \in A$ is defined as being a 4-uple $\langle J(a_i), P^-(a_i), I(a_i), P^+(a_i)\rangle$ where:

- $J(a_i) = \{a_j \in A | a_iJa_j\} = P_1(a_i)$,
- $P^-(a_i) = \{a_j \in A | a_jPa_i\} = P_2(a_i)$,
- $I(a_i) = \{a_j \in A | a_iIa_j\} = P_3(a_i)$,
- $P^+(a_i) = \{a_j \in A | a_iPa_j\} = P_4(a_i)$.

2.3. Distance

Due to the multicriteria nature of the problem, the concept of distance, so widely used in classification techniques, does not seem to be well suited here. This observation constitutes a fundamental barrier to the extension of famous clustering techniques, like the k-means algorithm. To avoid this bottleneck, our approach will be to define a distance between actions that will take into account their multicriteria nature.

Basically, the intuition behind this concept is that two actions will be as close as their profiles are alike.

Definition 3. Let $P(a_i)$ be the profile of a_i, the distance between two actions $a_i, a_j \in A$ is defined as follows:

$$d(a_i, a_j) = 1 - \frac{\sum_{k=1}^{4} |P_k(a_i) \cap P_k(a_j)|}{n} \tag{1}$$

See Appendix A for details on the proof that formula (1) is a distance.

2.4. Construction of the prototypes

With this definition of distance, extending the k-means algorithm to our problem now becomes much easier. The idea behind the method is to represent each potential cluster by a virtual central element. The actions are then assigned to the cluster with the nearest central element. Like that, new clusters are built and new central elements are determined. The process starts again until the cluster structure remains unchanged. In our case the definition of this central element (prototype) will be based on a voting procedure.

If the construction of the central elements seems quite intuitive for classic distances, in our case, it deserves more attention.

Definition 4. Let $\{a_{i_1}, \ldots, a_{i_p}\}$ be the p actions of the ith cluster. The profile of the ith central element, noted $P(c_i)$, will be determined by a voting procedure:

$$a_j \in P_k(c_i) \iff k = \arg\max \sum_{a_{i_l}} 1_{\{a_j \in P_k(a_{i_l})\}} \tag{2}$$

where $1_{\{A\}} = 1$ if condition A is true, 0 otherwise. If different values of k satisfy the previous condition, the final value will be randomly chosen.

The intuition behind this definition is that the profile of the ith central element is determined such that it is as close as possible to the profiles of the actions belonging to the ith class. This idea is confirmed by the following theorem:

Theorem 1. *Let $C_i = \{a_{i_1}, \ldots, a_{i_p}\}$ be a class of p actions and q a profile defined by a voting procedure. We have:*

$$q = \arg\min \sum_{j=1}^{p} d(a_{i_j}, q) \tag{3}$$

The proof of this theorem is developed in Appendix A.

3. MCDA clustering algorithm

Algorithm 1, here below, shows step by step, the procedures realized by the multicriteria clustering method developed in the previous section.

Being an extension of the k-means method, the previous algorithm suffers from the same weaknesses. Among these we can cite the fact that there is no uniqueness of results and that the initial conditions may strongly influence the classes structure, see for instance Bradley and Fayyad [5], and Bottou and Bengio [4]. Moreover some empirical tests have been conducted with the present algorithm. For more information the reader is referred to Montano-Guzman thesis [13]. However, it is worth noting that these few experiments have not led to conclusions different than those known for the classic version of the algorithm.

Algorithm 1. The MCDA clustering algorithm

Inputs: $A = \{a_1, a_2, \ldots, a_n\}$ set of actions, k the desired number of classes
Definition of $P(a_i)$ $\forall a_i$ such that we have the 4-uple
$\langle J(a_i), P^-(a_i), I(a_i), P^+(a_i)\rangle$
Randomly initialize k prototypes $(b_1, \ldots, b_k)$ such that $\forall j, \exists h\ b_j = a_h$
Each cluster C_j is associated with prototype b_j
repeat
  for all input vector a_l, where $l \in \{1, \ldots, n\}$ **do**
    Assign a_l to the cluster C_i with the nearest prototype b_i
    i.e. $d(a_l, b_i) \leqslant d(a_l, b_j)\ i, j \in \{1, \ldots, k\}$
  end for
  for all Clusters C_j, where $j \in \{1, \ldots, k\}$ **do**
    Update the prototype b_j to be the centroid of C_j
  end for
until The cluster membership no longer changes

4. Applications

As we mentioned in the introduction of this paper, the unsupervised learning techniques have many possible applications in different fields. In this section we will study two applications dedicated to financial problems: the Country Risk and the Firms Diagnosis Problems.

4.1. Country risk problem

Nowadays, being able to assess the creditworthiness of countries is a key problem for banks and international lending institutions. The definition of risk classes is a fundamental step, since institutions use them to determine the maximum bills outstanding authorized on a country and to evaluate the amount of reserve required.

In a previous paper, De Smet and Gilbart [6] have studied this problematic using an extension of the PROMETHEE method. The example treated in their paper was based on a set of 20 countries, namely: {Hong Kong, Greece, Israel, Slovenia, Czech Republic, Saudi Arabia, Chile, South Africa, Tunisia, Argentina, El Salvador, Croatia, Lebanon, Guatemala, Bulgaria, Peru, Zimbabwe, Honduras, Cote d'Ivoire, Ukraine}. To model the risk status of these countries, they have considered a set of eleven criteria based on economic, financial and political risks. A detailed analysis of their model may be found in De Smet and Gilbart [6] and in Gilbart [10]. Here below, we will exploit the preference structure on countries they have built to apply our algorithm.

To study the quality of this preference structure, let us first compute the Kendall's rank correlation coefficient between the Promethee II ranking (based on the considered preference structure) and the rankings of three official ratings: Institutional Investor, Euromoney and The Economist Intelligence Unit (see Table 1).

Before the application of our model, we need to specify the number of classes we want to obtain. As this information is not necessarily obvious, we will conduct experiments for a number of classes ranging from 1 to 9. Moreover a well-known feature of the k-means algorithm is the non-uniqueness of its results. To reduce this effect, once the number of classes has been fixed, we will apply 10 times the algorithm to the preference structure generated by the PROMETHEE methodology. Each time, the ratio between the sum of intra-class distances and the total sum of distances has been computed. This criteria represents the quality of

Table 1
Kendall's rank correlation coefficient between the Promethee II country ranking and three official rankings

Kendall's rank correlation	Promethee II	I.I.	Euromoney	EIU
Promethee II	1	0.832	0.789	0.632
I.I.		1	0.853	0.674
Euromoney			1	0.547
EIU				1

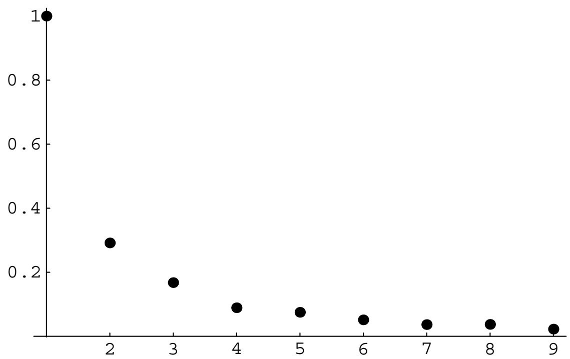

Fig. 1. Sum of intra-class distances divided by the total sum of distances for a number of classes varying from 1 to 9 (lowest ratio on 10 tests).

the considered partition. Among the 10 tests for each class, the lowest ratio has been kept.

Fig. 1 suggests that partitions in two or three classes are good compromises: the sum of intra-class distances divided by the total sum of distances is relatively low while the number classes is also small. Considering more classes will not lead to deeply increase the quality of the partition. On the other hand, considering a partition in two or three classes, instead of an unique class, permits to increase the quality in a significant way.

As we can see in Tables 2 and 3, the partitions in two or three classes are coherent with the rankings provided by Euromoney, Institutional Investor and EIU. If we consider two classes, noted A and B, we clearly observe that all the high-ranked countries belong to class A while low-ranked countries belong to class B. Moreover, the boundaries between classes remain satisfactory. Similar comments may be done in the case of a partition in three classes although the comparison with the EIU ranking is less significant. However, it is worth noting that this last ranking was already distinguishable on Table 1.

4.2. Diagnosis of firms

Diagnosis of firms problem has interested researchers and practitioners for many years. Altman [1], with the Discriminant Analysis, was one of the pioneers to analyze this problem with an analytical technique, in assessing the performance

Table 2
Country risk problem: Comparison between rankings of countries and their partition in two or three classes

Promethee 2	Two classes	Three classes	Euromoney	Two classes	Three classes
Hong Kong	A	A	Greece	A	A
Slovenia	A	A	Hong Kong	A	A
Greece	A	A	Israël	A	A
Czech Republic	A	A	Slovenia	A	A
Israël	A	A	Saudi Arabia	A	A
Chile	A	A	Chile	A	A
Saudi Arabia	A	A	Czech Republic	A	A
Croatia	B	B	South Africa	A	A
Tunisia	A	A	Tunisia	A	A
South Africa	A	A	Argentina	B	B
Argentina	B	B	El Salvador	A	B
Lebanon	B	B	Croatia	B	B
El Salvador	A	B	Guatemala	B	B
Peru	B	B	Lebanon	B	B
Guatemala	B	B	Bulgaria	B	C
Bulgaria	B	C	Peru	B	B
Cote d'Ivoire	B	C	Honduras	B	C
Honduras	B	C	Zimbabwe	B	C
Ukraine	B	C	Ukraine	B	C
Zimbabwe	B	C	Cote d'Ivoire	B	C

Table 3
Country risk problem: Comparison between rankings of countries and their partition in two or three classes

II	Two classes	Three classes	EIU	Two classes	Three classes
Greece	A	A	Chile	A	A
Hong Kong	A	A	Hong Kong	A	A
Chile	A	A	Slovenia	A	A
Slovenia	A	A	Czech Republic	A	A
Israël	A	A	Israël	A	A
Czech Republic	A	A	Greece	A	A
Saudi Arabia	A	A	Tunisia	A	A
South Africa	A	A	El Salvador	A	B
Tunisia	A	A	Peru	B	B
El Salvador	A	B	Bulgaria	B	C
Croatia	B	B	Saudi Arabia	A	A
Argentina	B	B	South Africa	A	A
Peru	B	B	Cote d'Ivoire	B	C
Guatemala	B	B	Lebanon	B	B
Bulgaria	B	C	Argentina	B	B
Lebanon	B	B	Honduras	B	C
Honduras	B	C	Croatia	B	B
Cote d'Ivoire	B	C	Guatemala	B	B
Ukraine	B	C	Ukraine	B	C
Zimbabwe	B	C	Zimbabwe	B	C

of the firms, different than the ratio analysis. After his seminal paper, different studies tried to develop appropriate models by applying various techniques including; multivariate discriminant analysis, logistic regression analysis, probit analysis, genetic algorithms, neural networks and decision trees as well as other statistical and multicriteria decision aid methods [2,9].

The purpose of this application is to explore the applicability of our multicriteria clustering

Table 4
Diagnosis of firms: Existing versus predicted classes structure—partition in two classes

	Predicted classes		Total
	C_1	C_2	
C_1: failed companies	8	1	9
C_2: not failed companies	6	24	30

Table 5
Diagnosis of firms: Existing versus predicted classes structure—partition in three classes

	Predicted classes			Total
	C_1	C_2	C_3	
C_1: failed companies	7	0	2	9
C_2: not failed companies	0	12	8	20
C_3: distressed companies	3	2	5	10

algorithm in the evaluation of firms. With the purpose to compare our results with those of previous studies, the model has been built using the ELECTRE III method, see Montano-Guzman thesis [13] for details.

The starting point of our analysis is the data studied in [8]. We consider a set of 39 firms on the basis of their financial evaluation. [1] First, we only consider failed (C_1) and not failed (C_2) firms. In a second test we add a third class for distressed companies (C_3). Results obtained with these two scenarios are summarized in Tables 4 and 5.

Tables 4 and 5 show a common structure between existing categories and those predicted by our algorithm. This is especially true for failed companies. On the other hand, differences for not failed and distressed companies must be analyzed carefully due to the temporal nature of the problem; a company that is currently not failed may be failed or distressed on the short term.

The model has also been tested with data obtained from Belfirst CD (2002). [2] We analyze 149 firms, all of these belonging to the Belgian building sector; 44 of these have failed and 105 are healthy

[1] Data are presented in [8].

[2] In this CD we can find the Company reports for the 290,000 companies incorporated under Belgian law and the 200 largest Luxembourg companies.

Table 6
Diagnosis of Belgian firms: Existing versus predicted classes structure—partition in two classes

	Predicted classes		Total
	C_1	C_2	
C_1: failed companies	36 (81.82%)	8 (18.18%)	44
C_2: not failed companies	2 (1.90%)	103 (98.10%)	105

firms. Table 6 summarizes the clustering results: the algorithm recovers 81.82% of failed firms while nearly all the "not failed" firms have been recovered.

5. Conclusions and future research

In this paper we developed an extension of the k-means algorithm to the multicriteria framework. The originality of this approach comes from the definition of a distance that takes into account the multicriteria nature of the problem.

The model introduced is independent from the way the decision maker builds his preferences (outranking methods, AHP, utility theory, ...). One more time, let us underline the fact that only outranking methods will lead to define a non-empty incomparability relation J. When applying other methods, the profiles of the actions will be restricted to P and I relations.

On the other hand, it is based on aggregated data and thus may loose some information. Furthermore, being an extension of the k-means method it suffers from the same bottlenecks; non uniqueness of the result, influence of initial conditions, ...

The algorithm has been tested on real-world data sets (country risk problem and diagnosis of firms) and shows encouraging results. Note that the use of the PROMETHEE method (country risk problem) and the ELECTRE III method (diagnosis of firms) to build preferences has been motivated from historical reasons: our goal was to recover data from previous studies to test our model. A comparison of these methods for these specific financial problems goes, of course, beyond the framework of this paper.

Future studies will be based on the application of the multicriteria distance introduced in this framework to other clustering or classification algorithms. Furthermore, the extension of this distance to cases where, for instance, the set of common incomparable actions are more weighted than the set of common indifferent actions, open new research directions. Finally, the application of the presented method to other real problems will allow us to confirm its coherence and to further analyze its distinctive features.

Appendix A. Proofs

Notations:

- $A = \{a_1, \ldots, a_n\}$,
- $ab = \{a_1 \cap b_1, a_2 \cap b_2, a_3 \cap b_3, a_4 \cap b_4\}$,
- $|a_i| =$ cardinality of a_i.

Theorem 2. *The application*

$$d : P \otimes P \to \left\{ \frac{h}{n} | h \in \{1, \ldots, n\} \right\} : (P(a), P(b)) \to d(a,b) = 1 - \frac{\sum_{i=1}^{4} |(ab)_i|}{n}$$

is a distance.

Proof

- $d(a,b) = d(b,a)$ by definition.
- $d(a,b) \geqslant 0$

$$d(a,b) \geqslant 0 \iff \sum_{i=1}^{4} |(ab)_i| \leqslant n,$$

$$\sum_{i=1}^{4} |(ab)_i| \leqslant \sum_{i=1}^{4} |a_i| = n.$$

- $d(a,b) = 0 \iff a = b$

If $a = b$, it follows from the definition of d that $d(a,b) = 0$.
If $d(a,b) = 0$ then

$$\sum_{i=1}^{4} |(ab)_i| = n.$$

As $|(ab)_i| \leqslant |a_i|$ and $|ab_i| \leqslant |b_i|$ it follows that

$$\sum_{i=1}^{4} |ab_i| = n = \sum_{i=1}^{4} |a_i| = \sum_{i=1}^{4} |b_i|.$$

And so $(ab)_i = a_i = b_i$, $\forall i$.

- $d(a,c) + d(c,b) \geqslant d(a,b)$

$$1 - \frac{\sum_{i=1}^{4} |(ac)_i|}{n} + 1 - \frac{\sum_{i=1}^{4} |(cb)_i|}{n} \geqslant 1 - \frac{\sum_{i=1}^{4} |(ab)_i|}{n}.$$

So, we have:

$$1 + \frac{\sum_{i=1}^{4} |(ab)_i|}{n} \geqslant \frac{\sum_{i=1}^{4} |(ac)_i|}{n} + \frac{\sum_{i=1}^{4} |(cb)_i|}{n}.$$

If $c = b$ or $c = a$ the bound is reached. Let us take $c = b$. If we swap k elements in the profile of c, we will always have

$$\sum_{i=1}^{4} |(ac)_i| \leqslant \sum_{i=1}^{4} |(ab)_i| + k.$$

But this transformation, leads also to

$$\sum_{i=1}^{4} |cb_i| = n - k. \qquad \square$$

Theorem 1. *Let $C = \{a_1, \ldots, a_q\}$ be a class of q actions and p a profile defined by a voting procedure. We have*

$$p = \arg\min \sum_{i=1}^{q} d(a_i, p).$$

Proof

$$\sum_{i=1}^{q} d(a_i, p) = \sum_{i=1}^{q} \left(1 - \frac{\sum_{j=1}^{4} |(a_i p)_j|}{n} \right) = q - \frac{1}{n} \sum_{i=1}^{q} \sum_{j=1}^{4} |(a_i p)_j|.$$

Let us consider any other profile $\hat{p}$ and let us proof that:

$$\sum_{i=1}^{q} \sum_{j=1}^{4} |(a_i \hat{p})_j| \leqslant \sum_{i=1}^{q} \sum_{j=1}^{4} |(a_i p)_j|,$$

$$\sum_{i=1}^{q}\sum_{j=1}^{4}|(a_i p)_j| = \sum_{i=1}^{q}\sum_{j=1}^{4}\sum_{x\in(p)_j} 1_{\{x\in(a_i)_j\}} = \sum_{j=1}^{4}\sum_{x\in(p)_j}\sum_{i=1}^{q} 1_{\{x\in(a_i)_j\}}$$

which is maximized by definition of the voting procedure. □

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