Analyzing the Structure of the Coupling Matrix with the Aid of the Associated Monotonic System *

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The subset of the "most distant" elements in a given set is determined and the classification of the elements generated by this subset is considered. The properties of the system of nested subsets obtained during the construction of the kernel of the monotonic system based on the coupling matrix are investigated.

1. Introduction

Practical experience with large-scale applications of automatic classification shows [1-5] that, first, the resulting classes widely differ in the mean density of objects and, second, the objects are distributed highly nonuniformly within the classes: there are "dense" and "sparse" regions, and some objects are very distant from the others, forming separate outlier classes as the number of is increased. This naturally leads to the problem of identifying, in a given set of coupled elements, the subset of elements, which are the "most isolated" in certain sense. Iterative application of this procedure (using the subset of elements from the previous stage instead of the original set in the analysis) would produce a family of classifications corresponding to the hierarchy of distances between the objects.

The article considers the problem of identifying the subset of "most distant" elements in a given set of coupled elements described by a coupling matrix. This problem may be considered as a modification of the well-known problem of automatic classification, since each of the identified elements may be treated as a representative of its class. Associating them with the nearest representative element does the assignment of the remaining elements to the different classes.

As in the automatic classification problem, the solution is reduced to extremizing a certain performance criterion. Our problem, however, has two distinctive features: first, a method can be constructed that gives an exact solution, producing the global extremum of the

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corresponding functional; second, the problem generates a classification with a number of classes, which is not known in advance.

While developing the subset of “maximally distant” elements, the initial set of coupled objects acquires a structure in the form of nested subsets partitioning the entire set into strata ordered by the strength of the coupling between the corresponding elements. This structure in a certain sense represents the most essential information contained in the original coupling matrix.

The concept of monotonic system introduced in [6] is central to the subject of this paper. Unlike [6], we consider a particular class of monotonic systems of functions on subsets of coupled elements. This concretization leads to a number of new propositions concerning the properties of the monotonic system and its subsystems.

The work consists of four sections. In Sec. 2 we consider the formal construction of the monotonic system on a given coupling matrix and present an exact formulation of the problem of identifying the subset of “maximally distant” elements. Section 3 describes an algorithm for the solution of this problem, and Sec. 4 discusses some properties of the solution, which are important for the purpose of interpretation. All theorems are proved in the Appendix.

2. Monotonic system on the coupling matrix

Consider a set W of N elements with a symmetric coupling matrix $A = \| a_{ik} \|_N^N$. It is assumed that all $i,k \in W$ we have

$$a_{ik} \geq 0,\ i \neq k,\ a_{ii} = 0. \tag{1}$$

Consider an arbitrary subset $H \subseteq W$. On every such subset we define a scalar numerical function of its elements

$$\pi(i,H) = \sum_{k \in H \setminus i} a_{ik} = \sum_{k \in H} a_{ik},\ \forall i \in H, \tag{2}$$

where $H \setminus i$ denotes the subset H without the element i, and the sum (2) is simplified using the assumption (1).

The number $\pi(i,H)$ assigned by this function to the element i on the subset H is called the weight of the element i on H. Thus the weight of each element of the subset H is equal to the sum of the coupling strength of this element with all the other elements of the subset.

The system $\pi(i,H)$ defined on the set of all subsets of the set W satisfied the condition

$$\pi(\beta,H\setminus\alpha)\le\pi(\beta,H),\ \forall\,\beta\in H\setminus\alpha\ \ (\beta\neq\alpha). \tag{3}$$

Such a system is called in [6] a monotonic system.

Let us now define on the set of all subsets of W a scalar function, which assigned to every subset H a number $F(H)$ by the following rule:

$$F(H)=\min_{i\in H}\pi(i,H),\ \forall\,H\subseteq W. \tag{4}$$

Then the problem of finding the subset of "maximally distant" elements may be stated as the problem of finding the global maximum of the functional $F(H)$:

$$F(H^*)=\max_{H\subseteq X}F(H)=\max_{H\subseteq X}\ \min_{i\in H}\ \pi(i,H). \tag{5}$$

The subset $H^*\subseteq W$ on which the function $F(H)$ takes its maximum is called in [6] the kernel of the monotonic system.

Suppose that the initial set W consists of several clusters of strongly coupled elements, where the coupling between different clusters is weak. Then the kernel H^* obtained from (5) consists of the "outliers" of these clusters, i.e., the elements with the weakest coupling between them.

Figure 1 shows an example of such a set of points on a plane, where the simple Euclidean distance is used as the measure of coupling between points i and j. Circles mark the kernel elements of this set. We see that, first, the kernel covers all the clusters that are sufficiently distant from the rest and, second, only the farthest outliers from each cluster are included in the kernel.

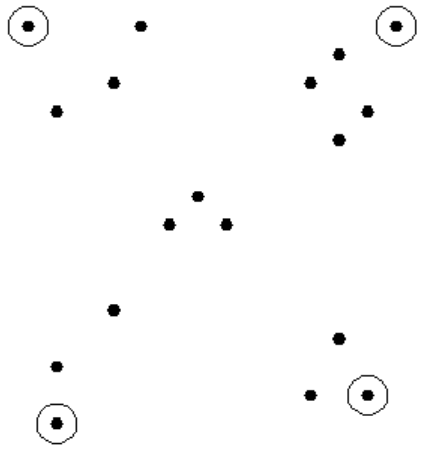

Fig. 1

Now let H^* be considered as the set of representatives of the different classes of elements of the initial set W. Then the simplest rule for assigning an arbitrary element $\alpha \in W$ to the class $W_S \subset W$ is given by the relation

$$a_{\alpha s} = \min_{i \in H^*} a_{\alpha i}. \tag{6}$$

Thus, unlike the traditional concept of representatives as the elements, which are the nearest in the mean to all the elements of corresponding classes (i.e., the center of their class), the representatives of classes in our case are elements lying far from the center of their class. Nevertheless, if the clusters in the initial set are sufficiently compact, both methods will apparently identify the same clusters. [1]

3. An algorithm for identifying the subsets of the most distant elements

The algorithm for the solution of the problem (5) is based on a procedure that constructs a so-called defining sequence of elements and isolates the largest kernel from the sequence, as proposed in [7].

The algorithm is described recursively.

[1] An another important requirement is that each of the clusters in the initial set should be sufficiently removed from all the rest.

Step 1. Set $H_1 = W$. Identify an element $\alpha_1 \in W$ such that

$$\pi(\alpha_1, W) = \min_{i \in X} \pi(i, W). \tag{7}$$

The element α_1 is the first element removed from the set W and the first element of the defining sequence. We denote its weight $\pi(\alpha_1, W)$ by δ_1.

This number will be used as the initial threshold for the comparison with the weights of the other elements in the subset $W \setminus \alpha_1$ that will be constructed in the next step. The comparison will be performed for the "removal" of other elements. The comparison threshold will be updated in subsequent steps.

Step k. After performing $(k-1)$ steps, we have the sequence of elements $\langle \alpha_1, \alpha_2, ..., \alpha_{k-1} \rangle$ [2] and the current comparison threshold is some number δ_{k-1}. Let H_k be the set of all the remaining elements of the set X at the beginning of the step k, i.e., those elements that have not been included in the defining sequence in the previous steps:

$$H_k = W \setminus \langle \alpha_1, \alpha_2, ..., \alpha_{k-1} \rangle. \tag{8}$$

Find an element α_k such that

$$\pi(\alpha_k, H_k) = \min_{i \in H_k} \pi(i, H_k) \tag{9}$$

and compare its weight with the current threshold δ_{k-1}. If

$$\pi(\alpha_k, H_k) \le \delta_{k-1} \tag{10}$$

and $k < N = |W|$, go to step $(k+1)$, without updating the threshold:

$$\delta_k = \delta_{k-1}. \tag{11}$$

Otherwise, i.e., if the inequality (10) is not true, update the threshold before continuing to the next step:

$$\delta_k = \pi(\alpha_k, H_k). \tag{12}$$

The algorithm stops when the entire initial set W has been exhausted, i.e., when all the elements have been arranged in such a defining sequence. The construction of the defining sequence induces the following sequence of subsets $\overline{H}$:

$$\langle H_1, H_2, ..., H_N \rangle, \tag{13}$$

where $H_1 = W$, $H_{k+1} = H_k \setminus \alpha_k$, and α_k is the k-th element of the defining sequence.

[2] The angular brackets $\langle , \rangle$, as in [7], denote ordered sets.

From the defining sequence $\langle \alpha_1, \alpha_2, ..., \alpha_N \rangle$ we select a special subsequence $\langle \alpha_{j_1}, \alpha_{j_2}, ..., \alpha_{j_p} \rangle$ whose elements correspond to the algorithm steps when the comparison threshold was updated. We may then write

$$\begin{aligned} &\delta_{j_1} = \delta_1 = \delta_2 = ... = \delta_{j_2-1}, \\ &\delta_{j_2} = \delta_{j_2+1} = \delta_{j_2+2} = ... = \delta_{j_3-1}, \\ &... \\ &\delta_{j_p} = \delta_{j_p+1} = \delta_{j_p+2} = ... = \delta_{j_N}. \end{aligned} \tag{14}$$

To simplify the subsequent analysis, we introduce special notation for this subsequence of elements and the associated subsequence of sets:

$$\overline{\gamma} = \langle \gamma_1 = \alpha_{j_1}, \gamma_2 = \alpha_{j_2}, ..., \gamma_p = \alpha_{j_p} \rangle, \tag{15}$$

$$\overline{\Gamma} = \langle \Gamma_1 = H_{j_1}, \Gamma_2 = H_{j_2}, ..., \Gamma_p = H_{j_p} \rangle. \tag{16}$$

The numerical sequence of the thresholds is similarly transformed:

$$\overline{u} = \langle u_1 = \delta_{j_1}, u_2 = \delta_{j_2}, ..., u_p = \delta_{j_p} \rangle. \tag{17}$$

Let H^* be the corresponding subset $\Gamma_p = H_{j_p}$, i.e., the subset of elements included in the defining sequence after the last change of the threshold in the j_p-th step, together with the element γ_p. It is shown in [7] that the function $F(H)$ attains its global maximum on the set H^*. Thus H^* is the subset of the "most distant" elements" sought in our problem.

Computationally, this procedure reduces to successive calculation of the values of the function $\pi(i, H_k)$, $\forall i \in H_k$ from the known values of the function $\pi(i, H_{k-1})$. From the definition of the function $\pi(i, H)$ in (2) we have the following computational formula:

$$\pi(i, H_k) = \pi(i, H_{k-1}) - a_{i\alpha_{k-1}}. \tag{18}$$

We see from this formula that the algorithm is computationally fairly simple and therefore may be applied to large systems of coupled elements.

The relation (18) also provides a visual expression of the monotonic property (3) of the relevant system of functions, since for coupling matrix satisfying the condition (1), the re-

moval of any element α_k from an arbitrary set subset H_k may only reduce the weights of the remaining elements in H_k.

4. The properties of the monotonic system of a coupling matrix

As we have noted above, an important property of the algorithm is that, simultaneously with determining the subset of the "most distant" elements, it produces a system of nested subsets $\langle \Gamma_j \rangle$, $j = 1,2,...,p$, the last of which Γ_p is the sought kernel. These sets have special properties.

Two general comments, which follow directly from the construction of the solution algorithm, should be made at this point. First, the sequence of the threshold values generated by the algorithm is strictly ordered:

$$u_1 < u_2 < ... < u_j < u_{j+1} < ... < u_p, \tag{19}$$

where

$$u_j = \min_{i \in \Gamma_j} \pi(i, \Gamma_j) = \min_{i \in \Gamma_j} \sum_{k \in \Gamma_j} a_{ik}. \tag{20}$$

Second, the sets in the sequence $\overline{\Gamma}$ are points of the local extrema (maxima) of the function F in the sequence of sets $\overline{H}$:

$$F(\Gamma_j) = \max_{\Gamma_j \supset H \supset \Gamma_{j+1}} F(H), \ \forall H \in \overline{H}, \ j = 1,2,...,p-1 \tag{21}$$

or

$$\begin{array}{l|l} F(H) \le F(\Gamma_j) = u_j & \forall H \in \overline{H}, \Gamma_j \supset H \supset \Gamma_{j+1}, \\ F(H) < F(\Gamma_{j+1}) = u_{j+1} & j = 1,2,...,p-1. \end{array} \tag{22}$$

Moreover, as noted in [7], the relations (21) and (22) are true for every subset G, $\Gamma_j \supset G \supset \Gamma_{j+1}$, which is not necessarily a member of the sequence of subsets $\overline{H}$.

Theorem 1. For every proper subset G, $\Gamma_j \supset G \supset \Gamma_{j+1}$, we have

$$\begin{array}{ll} \text{a)} & F(G) \le F(\Gamma_j) = u_j \qquad \Gamma_j \supset G \supset \Gamma_{j+1}, \\ \text{b)} & F(G) < F(\Gamma_{j+1}) = u_{j+1} \quad j = 1,2,...,p-1. \end{array} \tag{23}$$

It follows from Theorem 1 that the sequence of sets $\overline{\Gamma}$ is a sequence of points of strictly increasing local maxima of the function F. The last of the maxima in this sequence is also the global maximum.

The function $F(H)$ thus has a very simple structure: it has a total of $p \le N = |W|$ local maxima. This simplicity, which is a consequence of the monotonicity of the system, makes it possible to construct a fast algorithm for the solution of the problem (5): the algorithm in this case is a simple procedure enumerating all the local maxima of the function $F(H)$.

Because of this property, the kernel algorithm of a monotonic system can be used to solve the initial problem with additional constraints. Thus, in particular, we can carry out a special enumeration of the key elements, which must be included in the resulting subset; in other cases, the admissible size of the sought subset may be specified (the desired range). In both cases, the solution of the problem is the smallest set Γ_j satisfying the corresponding constraint, e.g., the smallest set Γ_j including the specified key elements.

For purpose of interpretation of the results, it is desirable to have performance criteria that provide quantitative measures of the distance of the kernel elements H^* and the homogeneity of their relative distribution. Two such criteria are the functions $F(\Gamma_p)$ and $Q(\Gamma_p)$, respectively, which are defined as follows:

$$F(\Gamma_p) = \min_{i \in \Gamma_p} \sum_{k \in \Gamma_p} a_{ik}, \tag{24}$$

$$Q(\Gamma_p) = \max_{H \subset \Gamma_p} \max_{i \in \Gamma_p \setminus H} \sum_{k \in H} a_{ik}, \; H \in \overline{H}, \; (H \subset \Gamma_p, \; \Gamma_p \setminus H \neq \varnothing). \tag{25}$$

As we have noted, $F(\Gamma_p)$ identifies a special element, the center of the kernel, whereas $Q(\Gamma_p)$ specifies proper part H' of the kernel Γ_p, and from the monotonicity property it follows that the element $\alpha \in \Gamma_p \setminus H'$, such that $\sum_{k \in H'} a_{\alpha k} = \max_{i \in \Gamma_p \setminus H'} \sum_{k \in H'} a_{\alpha k}$ immediately precedes the first element of H' in the defining sequence.

The usefulness of $F(\Gamma_p)$ and $Q(\Gamma_p)$ as the distance measure of the kernel elements and the measure of homogeneity of their relative distribution follows from the basic properties, as formulated in Theorem 2 and 3.

Theorem 2. The measure of kernel homogeneity does not exceed the threshold value $u_p = F(\Gamma_p)$:

$$Q(\Gamma_p) \le \min_{i \in \Gamma_p} \sum_{k \in \Gamma_p} a_{ik} . \tag{26}$$

Theorem 3. The minimum sum of the coupling strength between a given element of the set and all the other elements of the set, i.e., the threshold value $u_p = F(\Gamma_p)$, is not less than the maximum coupling strength between any two elements of the set X:

$$F(\Gamma_p) \ge \max_{i,k \in W} a_{ik} . \tag{27}$$

Unlike Theorem 2, which in a certain sense guarantees "density" of the set Γ_p, Theorem 3 imposes an essential lower bound on the mean coupling strength, i.e., on the "distance" of the elements in this set.

The measures of distance and homogeneity (density) introduces in Theorems 2 and 3 for the elements of the kernel (the set on which the function $F(H)$ has its global maximum) can be generalized to evaluate all the local extrema of this function. The corresponding criteria are similarly defined:

$$F(\Gamma_j) = \min_{i \in \Gamma_j} \sum_{k \in \Gamma_j} a_{ik} , \ j = 1,2,\ldots, p-1, \tag{28}$$

$$Q(\Gamma_j) = \max_{H} \max_{i \in \Gamma_j \setminus H} \sum_{k \in H} a_{ik} , \ \Gamma_j \supset H \supset \Gamma_{j+1}, \ H \in \overline{H} , \ j = 1,2,\ldots, p-1. \tag{29}$$

Theorem 4. For every set Γ_j,

$$Q(\Gamma_j) \le \min_{i \in \Gamma_j} \sum_{k \in \Gamma_j} a_{ik} , \ j = 1,2,\ldots, p-1. \tag{30}$$

Theorem 5. For every set Γ_j, the minimal sum of the coupling strength of a given element with all the other elements of the set, i.e., the threshold value $u_j = F(\Gamma_j)$, is not less that the maximum coupling strength between any two elements i and k, which do not belong to Γ_{j+1}, i.e., $i,k \in W \setminus \Gamma_{j+1}$,

$$F(\Gamma_j) \ge \max_{i,k \in W \setminus \Gamma_{j+1}} a_{ik} , \ j = 1,2,\ldots, p-1. \tag{31}$$

Theorems 4 and 5 justify using the local extrema of the function F, i.e., the sets $\langle \Gamma_j \rangle$, $j = 1,2,\ldots, p-1$, as an acceptable solution for the subset of the "most distant" elements in problems with additional constraints. The measures of "distance" and homogeneity of the elements introduced in these theorems and their comparison with the corresponding criteria for the global maximum indicate to what extent the ideal solution is distorted by the additional constraints.

In conclusion, let us consider Theorem 6, which establishes that sets $\langle \Gamma_j \rangle$, $j = 1,2,\ldots, p-1$, are in a certain sense also the local extrema of the functional defined as the mean coupling strength of the elements in the subset.

Theorem 6. Let

$$f(H) = \frac{1}{|H| \cdot (|H| - 1)} \cdot \sum_{i,k \in H} a_{ik}\ ,\ \forall\, H \subseteq W\ . \tag{32}$$

Then the following propositions are true:

A. Every subset $H \subset \Gamma_j$, $j = 1,2,\ldots, p-1$ with $|H| = |\Gamma_{j+1}|$ elements, which differs from Γ_{j+1} at most in one element, satisfies the inequality

$$f(H) < f(\Gamma_{j+1}). \tag{33}$$

B. Every subset $H \subset \Gamma_j$, $j = 1,2,\ldots, p-1$ with $|H| = (|\Gamma_{j+1}| + 1)$ elements, which contains the set Γ_{j+1}, i.e., $H \supset \Gamma_{j+1}$, also satisfies the inequality (33).

The monotonicity properties of the system based on the coupling matrix provide rich opportunities for meaningful interpretation.

Remark. The formal statement of the problem for the subset of the "most distant" elements and the corresponding solution algorithm are preserved when the element a_{ik} of the coupling matrix is interpreted as a measure of proximity or goodness of fit (and not as a measure of distance). The relevant problem in this case is to isolate a subset of coupled elements from the set X, which are the "nearest" in the sense of (5).

APPENDIX

Proof of Theorem 1. The validity of inequality a) is proved by contradiction.

Suppose there is a subset G, $\Gamma_j \supset G \supset \Gamma_{j+1}$ such that

$$F(G) > F(\Gamma_j) = u_j. \tag{A.1}$$

In the sequence $\overline{H}$ there is a minimal subset $H_t \in \overline{H}$, $H_t \subseteq \Gamma_j$, such that $H_t \supseteq G$. Clearly, $\alpha_t \in G$, where $\alpha_t \in H_t$, $\alpha_t \notin H_{t+1}$.

Let $\alpha_g \in G$ be the minimal-weight element in G, i.e.,

$$\pi(\alpha_g, G) = \min_{i \in G} \pi(i, G). \tag{A.2}$$

Then

$$\pi(\alpha_t, G) \geq \pi(\alpha_g, G) = F(G). \tag{A.3}$$

From the monotonicity property we have

$$\pi(\alpha_t, H_t) \geq \pi(\alpha_g, G), \text{ since } H_t \supseteq G. \tag{A.4}$$

Hence, using (A.1) and (A.3), we obtain

$$\pi(\alpha_t, H_t) > F(\Gamma_j) = u_j. \tag{A.5}$$

On the other hand, from the construction of the defining sequence, for $H_t \subseteq \Gamma_j$, $\alpha_t \in H_t$, $\alpha_t \notin H_{t+1}$ we have

$$\pi(\alpha_t, H_t) \leq u_j. \tag{A.6}$$

The last two inequalities contradict one another, which proves the inequality a).

The validity of the inequality b) in Theorem 1 follows from relations (19),(20) and the inequality a). ■

Proof of Theorem 2. Suppose the proposition of Theorem 2 is false, i.e., there is an element $\alpha \in \Gamma_p \setminus H$ such that

$$\sum_{k \in H} a_{ik} > \min_{i \in \Gamma_p} \sum_{k \in \Gamma_p} a_{ik}. \tag{A.7}$$

The element α belongs to $\Gamma_p \setminus H$, i.e., it does not belong to H: $\alpha \notin H$. Let H_t be the smallest subset in the sequence $\overline{H}$ containing the element α, i.e., $\alpha \in H_t$, but $\alpha \notin H$. Clearly, $H_t \supset H$. By (10) the elimination of α from H_t is possible only if $\pi(\alpha, H_t) \le u_p$, i.e.,

$$\sum_{k \in H_t} a_{ik} \le u_p, \tag{A.8}$$

since u_p is the last threshold value, which is not updated until the end. Since $H_t \supset H$, we have

$$\sum_{k \in H} a_{ik} \le \sum_{k \in H_t} a_{ik}. \tag{A.9}$$

Hence

$$\sum_{k \in H} a_{ik} \le \min_{i \in \Gamma_p} \sum_{k \in \Gamma_p} a_{ik}. \tag{A.10}$$

The inequality (A.10) contradicts the assumption (A.7). ■

Proof of the Theorem 3. The function $F(H)$ attains its global maximum on $\Gamma_p = H^*$. i.e.,

$$F(H^*) \ge F(H) \ \ \forall H \subseteq W. \tag{A.11}$$

Therefore, this inequality holds for all two-element subsets in W, including some $\{\alpha, \beta\}$, such that $a_{\alpha\beta} = \max_{i,k \in W} a_{ik}$. Now since

$$F(\{\alpha, \beta\}) = \min_{i \in \{\alpha, \beta\}} \pi(i, \{\alpha, \beta\}) = a_{\alpha\beta}, \tag{A.12}$$

the truth of the inequality (27) is established.

Theorems 4 and 5 are proved along the same lines as Theorem 2 and 3.

Proof of the Theorem 6. Both propositions of Theorem 6 follow from Theorem 4 and the inequality (19). Indeed,

$$\max_{i \in \Gamma_j \setminus \Gamma_{j+1}} \sum_{k \in \Gamma_{j+1}} a_{ik} \le u_j < u_{j+1} = \min_{i \in \Gamma_{j+1}} \sum_{k \in \Gamma_{j+1}} a_{ik}. \tag{A.13}$$

The inequality (A.13) means that even if the element $\gamma_{j+1} \in \Gamma_{j+1}$ with the minimal sum of coupling strengths with the elements of the set Γ_{j+1} is replaced by the element $\alpha \in \Gamma_j \setminus \Gamma_{j+1}$ with the maximal sum of coupling strengths with the elements of Γ_{j+1}, the total sum of coupling strengths of the resulting subset, and hence the average coupling strength between pairs of elements, may only diminish (proposition A).

Adding to the subset Γ_{j+1} any of elements from $\Gamma_j \setminus \Gamma_{j+1}$ will increase the total sum of coupling strength between the elements of the subset $H \subset \Gamma_j$, $|H| = |\Gamma_{j+1}| + 1$, but nevertheless decrease the average coupling strength, which also follows from the inequality (A.13) (proposition B). ■

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