

AN ALGORITHM FOR FUZZY CLUSTERING BASED ON FUZZY RELATIONS

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ABSTRACT

In this paper, some properties of the fuzzy equivalence matrices are discussed. On this basis, we propose a simple and convenient method of hierarchical clustering by a fuzzy similar matrix R on the patterns set X .

KEYWORDS: Fuzzy equivalence matrix, Equivalence level, Equivalence point.

1. INTRODUCTION

S. Tamura et al. [1] described a hierarchical clustering scheme based on a fuzzy equivalence relation on a patterns set X . To start with, we give a fuzzy relation R on X by calculating the coefficients of similarity or the distances of each pair of patterns that is taken from the population of patterns to be classified. A fuzzy relation matrix $R = [r_{ij}]_{n \times n}$ may express a fuzzy relation when X is a finite set. R is called a similar matrix if it satisfies the following two conditions,

(1°). reflexivity: $r_{ii} = 1$,

(2°). symmetry: $r_{ij} = r_{ji}$,

where $0 \leq r_{ij} \leq 1$, $i, j = 1, 2, \dots, n$. A fuzzy matrix R is called an equivalence matrix if it is similar and satisfies the condition

(3°). transitivity: $R \circ R \leq R$,

where $R \circ R = A \hat{=} [a_{ij}] \Leftrightarrow a_{ij} = \bigvee_{l=1}^n (r_{il} \wedge r_{lj})$. (1)

Let R be an equivalence matrix. Because R is symmetric, we have

$$R \circ R = A \Leftrightarrow a_{ij} = \bigvee_{l=1}^n (r_{il} \wedge r_{jl}) \quad (2)$$

and $R \circ R \geq R$, thus the condition (3°) may be replaced by

$$(3^*) \quad R \circ R = R. \quad (3)$$

Using an equivalence relation on the patterns set X , we can

classify the present population of the patterns into some classes. However, in many experiments of the classification, the fuzzy relation matrix R obtained is a similar matrix, not an equivalence matrix. An improvement is to compute the transitive closure R^* for the fuzzy similar matrix R . It had been proved that transitive closure of a fuzzy similar matrix R can be obtained by calculating R^{2^k} in finite steps. Obviously, the computing process is complicated when the order of R is high.

A great amount of the works have been done on the basis of Tamura's scheme, such as Dunn [2] proposed a method of maximal spanning trees and Zhao ruhuai [4] a net-making method. In this paper, we will propose a simple and convenient method of hierarchical clustering by fuzzy similar matrix R on the patterns set X . It is shown that procedure is superior to algorithms of [1], [2], [4] with regard to both computing time and storage requirements.

2. PROPERTIES OF FUZZY EQUIVALENCE MATRICES

We suppose that fuzzy relation matrix R is similar through the paper.

Definition 2.1 The entry r_{ij} of a fuzzy similar matrix $R = [r_{ij}]_{n \times n}$ is called a equivalence level, if r_{ij} ($i \neq j$) is a maximal element in the i -th row of R except the diagonal element r_{ii} .

Definition 2.2 Let $k \times k$ ($k < n$) matrix $R_{\langle k \rangle}$ be a submatrix of the $n \times n$ matrix R , where

$$R = \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ r_{21} & r_{22} & \cdots & r_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ r_{n1} & r_{n2} & \cdots & r_{nn} \end{bmatrix} \quad \text{and} \quad R_{\langle k \rangle} = \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1k} \\ r_{21} & r_{22} & \cdots & r_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ r_{k1} & r_{k2} & \cdots & r_{kk} \end{bmatrix},$$

we call $R_{\langle k \rangle}$ a main submatrix of R .

Proposition 2.1 If $n \times n$ fuzzy matrix R is equivalent, then each order main submatrices $R_{\langle 1 \rangle}$, $R_{\langle 2 \rangle}$, \dots , $R_{\langle n-1 \rangle}$ are equivalent.

Proof: Suppose that $R_{\langle s \rangle}$ does not satisfy transitivity ($s < n$), then there are at least one r_{ij} ($1 \leq i \neq j \leq s$) such that

$$\text{i.e. } \bigvee_{l=1}^s (r_{il} \wedge r_{jl}) > r_{ij}$$

$$\text{i.e. } \bigvee_{l=1}^n (r_{il} \wedge r_{jl}) \geq \bigvee_{l=1}^s (r_{il} \wedge r_{jl}) > r_{ij} \quad (4)$$

(4) shows that R is not equivalent.

Proposition 2.2 If a fuzzy matrix R is equivalent, then we have

$$r_{ij} = r_{ik} \wedge r_{kj}$$

for any $i, j = 1, 2, \dots, n$, $i \neq j$, where r_{ik} is the equivalence level of R.

Proof: Since R is equivalent, then we have

$$r_{ij} = \bigvee_{l=1}^n (r_{il} \wedge r_{lj}) = \bigvee_{l \neq k} (r_{il} \wedge r_{lj}) \vee (r_{ik} \wedge r_{kj}) \geq r_{ik} \wedge r_{kj}$$

i.e. $r_{ij} \geq r_{ik} \wedge r_{kj}$. (5)

And $r_{kj} = \bigvee_{l=1}^n (r_{kl} \wedge r_{lj}) = \bigvee_{l \neq i} (r_{kl} \wedge r_{lj}) \vee (r_{ki} \wedge r_{ij}) \geq r_{ki} \wedge r_{ij}$
 i.e. $r_{kj} \geq r_{ki} \wedge r_{ij}$. Because $r_{ki} = r_{ik}$ is the equivalence level of R, then we have $r_{kj} > r_{ij}$, hence

$$r_{ij} \leq r_{ik} \wedge r_{kj} \quad (6)$$

(5) and (6) imply $r_{ij} = r_{ik} \wedge r_{kj}$.

Proposition 2.3 Let $n \times n$ main submatrix $R_{<n>}$ of $(n+1) \times (n+1)$ fuzzy matrix R be equivalent, and R be reflexive and symmetric. If entries r_{ij} of R satisfy the following equalities

$$r_{ij} = r_{ik} \wedge r_{kj}, \quad i, j = 1, 2, \dots, n+1, \quad i \neq j, \quad i \neq k,$$

then R is also equivalent, where r_{ik} is the equivalence level of R.

Proof: By way of a contradiction suppose that $(n+1) \times (n+1)$ matrix R is not equivalent, i.e. there exist i, j such that

$$r_{ij} \neq \bigvee_{l=1}^{n+1} (r_{il} \wedge r_{lj}) = \bigvee_{l=1}^n (r_{il} \wedge r_{lj}) \vee (r_{i, n+1} \wedge r_{n+1, j}).$$

Since $r_{ij} = \bigvee_{l=1}^n (r_{il} \wedge r_{lj})$, hence

$$r_{ij} < r_{i, n+1}, \quad r_{ij} < r_{n+1, j} = r_{j, n+1}. \quad (7)$$

We consider the following two cases respectively.

1. There are at least an equivalence level of the $(n+1)$ th column of R at $r_{i, n+1}$ or $r_{j, n+1}$, where $i \neq n+1, j \neq n+1$.

Suppose that $r_{i, n+1}$ ($i \neq n+1$) is an equivalence level of the $(n+1)$ th column of R. Since R is symmetric, then $r_{i, n+1} = r_{n+1, i}$, $r_{j, n+1} = r_{n+1, j}$. By the assumptions, we have $r_{n+1, j} = r_{n+1, i} \wedge r_{ij}$, i.e. $r_{j, n+1} = r_{i, n+1}$

$\wedge r_{ij}$, which contradicts (7).

2. Both $r_{i,n+1}$ and $r_{j,n+1}$ are not equivalence level of the $(n+1)$ th column of R . where $i \neq n+1, j \neq n+1$.

Suppose that $r_{t,n+1}$ is an equivalence level of R , $t \neq i, t \neq j$. By symmetry and the assumptions, we have

$$r_{i,n+1} = r_{t,n+1} \wedge r_{it},$$

$$r_{j,n+1} = r_{t,n+1} \wedge r_{jt},$$

because $r_{t,n+1} > r_{i,n+1}$, $r_{t,n+1} > r_{j,n+1}$, thus $r_{it} = r_{i,n+1}$, $r_{jt} = r_{j,n+1}$, which contradicts (7).

This completes our proof.

Proposition 2.4 A necessary and sufficient condition that a fuzzy similar matrix R is equivalent is that for any $i, j = 1, 2, \dots, s$, $i \neq j$ and $s = 1, 2, \dots, n$, each order main submatrices $R_{\langle s \rangle}$ satisfy the following

$$r_{ij} = r_{ik} \wedge r_{kj}$$

where r_{ik} is the equivalence level of $R_{\langle s \rangle}$.

Proof: The proof is obvious.

Proposition 2.5 The entries of a fuzzy matrix R^k are denoted by $r_{ij}^{(k)}$, where $R^2 = R \circ R$, $R^k = R^{k-1} \circ R$, $k = 2, 3, \dots$. If r_{ij} is an equivalence level of R , then for any positive integer k , r_{ij} is still an equivalence level of R^k , i.e. $r_{ij}^{(k)} = r_{ij}$.

Proof: Since $r_{il} \leq r_{ij}$ ($l \neq i, l \neq j$), by (1), then we have $r_{il}^{(k)} \leq r_{ij}$. Because $r_{ij}^{(2)} = \bigvee_{l=1}^n (r_{il} \wedge r_{lj}) = \bigvee_{l \neq i} (r_{il} \wedge r_{lj}) \vee r_{ij} \geq r_{ij}$, thus $r_{ij}^{(2)} = r_{ij}$, and r_{ij} is still an equivalence level of R^2 . By the induction method, we can easily obtain the result.

Definition 2.3 Let r_{ij} be an equivalence level of the fuzzy similar matrix R , the pair (i, j) is called an equivalence point of R (in fact, the pair (i, j) is a point on Cartesian product space $X \times X$ when we regard R as a fuzzy subset on $X \times X$).

From Definition we easily see that if (i, j) is an equivalence point, then (j, i) is also an equivalence point, where $i \neq j$. Generally, (i, j) and (j, i) are regarded as the same equivalence point.

Definition 2.4 Let $u_1 = (a_1, a_2)$, $u_2 = (b_1, b_2)$ be two equivalence points of R . We call that u_1 and u_2 are in same fuzzy equivalence chain iff $\exists 1 \leq i, j \leq 2$ such that $a_i = b_j$.

We call that equivalence point $(i, k_1), (k_1, k_2), \dots, (k_{m-1}, k_m), (k_m, j)$ form a fuzzy equivalence chain, denoted by $e = \{i, k_1, \dots, k_m, j\}$.

Definition 2.5 Suppose all equivalence points of $n \times n$ fuzzy matrix R form m equivalence chains e_1, e_2, \dots, e_m whose union

$$\bigcup_{i=1}^n e = \{1, 2, \dots, n\} .$$

Let $E = \{e_1, e_2, \dots, e_m\}$, $R^{<2>} = [r_{ij}^{<2>}]$ be a fuzzy similar relation matrix on $E \times E$, where $1 \leq i, j \leq m$, $m \leq \lfloor \frac{n}{2} \rfloor$, $r_{ij}^{<2>}$ is a measure of similarity between two equivalence chains $e_i = \{i_1, i_2, \dots, i_{k_1}\}$ and $e_j = \{j_1, j_2, \dots, j_{k_2}\}$, we take that

$$r_{ij}^{<2>} = \bigvee_{\substack{u=1, \dots, k_1 \\ v=1, \dots, k_2}} r_{i_u, j_v} \quad , \quad r_{kk}^{<2>} = 1 \quad , \quad (k=1, 2, \dots, m).$$

where r_{i_u, j_v} are the entries of the matrix R . The equivalence points of R are called the second order equivalence points of R , denoted by $(i, j)_2$.

Similarly, the fuzzy similar matrix $R^{<N>}$ can be constituted by the equivalence chains of $R^{<N-1>}$. The equivalence points of $R^{<N>}$ are called the N -th order equivalence points, $N = 1, 2, \dots$, denoted by $(i, j)_N$.

Proposition 2.6 If all equivalence points of $n \times n$ fuzzy similar matrix R form an equivalence chain, then each entries of the transitive closure $R^* = [r_{ij}^*]$ for fuzzy similar matrix R are all equivalence levels of R except $r_{ii}^* = 1, i = 1, 2, \dots, n$.

Proof: We only show that r_{ij}^* is equal to one of the equivalence levels of R , for any $i, j = 1, 2, \dots, n, i \neq j$.

Let $r_{i, k_1}, r_{k_1, k_2}, \dots, r_{k_l, j}$ be the equivalence levels relatively to equivalence points $(i, k_1), (k_1, k_2), \dots, (k_l, j)$ of R . By Proposition 2.5, we have $r_{i, k_1}^* = r_{i, k_1}, r_{k_1, k_2}^* = r_{k_1, k_2}, \dots, r_{k_l, j}^* = r_{k_l, j}$, and $(i, k_1)_*, (k_1, k_2)_*, \dots, (k_l, j)_*$ are the equivalence points of R^* . For any $i, j = 1, 2, \dots, n, i \neq j$, by Proposition 2.2 we have the following

$$\begin{aligned} r^* &= r_{i, k_1} \wedge r_{k_1, j} \\ &= r_{i, k_1} \wedge r_{k_1, k_2} \wedge r_{k_2, j} \\ &\quad \dots \dots \dots \\ &= r_{i, k_1} \wedge r_{k_1, k_2} \wedge \dots \wedge r_{k_{l-1}, k_l} \wedge r_{k_l, j} \end{aligned}$$

which means that r_{ij}^* is equal to one of the equivalence levels

$r_{i_{k_1}}, \dots, r_{k_l, j}$ of R .

Proposition 2.7 Let $R^* = [r_{ij}^*]_{n \times n}$ be the transitive closure of similar matrix $R = [r_{ij}]_{n \times n}$. For any $i, j = 1, 2, \dots, n, i \neq j$, there are at least a k such that $r_{ij}^* = r_{uv}^{<k>}$, where $r_{uv}^{<k>}$ is a k -th order equivalence level of R .

Proof: First, we discuss a simple case. Let all first order equivalence points of $n \times n$ fuzzy similar matrix R form two chains $e_1 = \{1, 2, \dots, m\}$, $e_2 = \{m+1, m+2, \dots, n\}$ (If we obtain $e'_1 = \{i_1, i_2, \dots, i_m\}$, $e'_2 = \{i_{m+1}, i_{m+2}, \dots, i_n\}$, we can reorder the patterns of X such that $i_k \rightarrow k$). We denote that

$$U_{1,2} = \{ r_{ij} \mid r_{ij} \text{ is the entries of } R, i=1,2,\dots,m, j=m+1, m+2,\dots,n \},$$

$$M = \{ r_{ij} \mid (i,j) \text{ is first order equivalence points, } i,j=1,2,\dots,n \},$$

$$R_{<m>} = [r_{ij}]_{m \times m}, i,j=1,2,\dots,m.$$

$$R'_{<n-m>} = [r_{ij}]_{(n-m) \times (n-m)}, i,j=m+1,m+2,\dots,n.$$

i.e. $R_{<m>}$ and $R'_{<n-m>}$ are submatrices of $R = [r_{ij}]_{n \times n}$.

1. When $r_{ij} \in M$ and $r_{ij} \in U_{1,2}$, we can see that r_{ij} is an entry of $R_{<m>}$ or $R'_{<n-m>}$ by the symmetry. Because $R_{<m>}$ and $R'_{<n-m>}$ satisfy the conditions of Proposition 2.6, hence $r_{ij}^* \in M$.

2. Let r_{ij} be a maximal entry on $U_{1,2}$. For any l , it is impossible that r_{ij} and r_{lj} in the expression $r_{ij}^{(2)} = \bigvee_{l=1}^n (r_{il} \wedge r_{lj})$ are all elements of M . And there exists an element in $\{r_{il}, r_{lj}\}$ for each $l=1,2,\dots,n$ is the element of $U_{1,2}$. Hence we can easily see that $r_{ij}^{(2)} = r_{ij}$, and $r_{ij}^{(k)} = r_{ij}$ for any k .

Let $r_{ik} \in M$, $r_{ij} \in U_{1,2}$. By Propositions 2.2 and 2.5, we have $r_{ij} = r_{kj}$, because $r_{ij} < r_{ik}$, $j = m+1, m+2, \dots, n$, hence all row vectors of the submatrix $R_U = [\alpha_{ij}]$ ($\alpha_{ij} \in U_{1,2}$) of R are the same. By the symmetry, all columns are the same. This shows that the entries of R_U are all the same, they are just the equivalence levels of second order equivalence points of R .

Second, we discuss the generally case. Let all first order equivalence points of $n \times n$ matrix R form k chains $e_1 = \{1, 2, \dots, m_1\}$, $e_2 = \{m_1 + 1, m_1 + 2, \dots, m_2\}$, \dots , $e_k = \{m_{k-1} + 1, m_{k-1} + 2, \dots, m_k\}$, where

$m_1 + m_2 + \dots + m_k = n$. We denote that

$$U_{l,t} = \{ r_{ij} \mid r_{ij} \text{ is the entries of } R, i \in e_l, j \in e_t \}.$$

1'. If $r_{ij} \in M$ and $r_{ij} \in U_{l,t}$, we have $r_{ij}^* \in M$ similar to 1.

2'. For any $l, t = 1, 2, \dots, k, l \neq t$, the elements of $U_{l,t}$ take the same value similar to 2.

3'. Let $r_{ij} \in U_{l,t}$ and for any $r_{ik} \in U_{u,v}$ we have $r_{ij} \geq r_{ik}$. because for any l it is impossible that r_{il} and r_{ij} in the expression $r_{ij}^{(2)} = \bigvee_{l=1}^n (r_{il} \wedge r_{lj})$ are all elements of M , hence we have $r_{ij}^{(2)} = r_{ij}$. By analogies, $r_{ij}^{(k)} = r_{ij}$ for any positive integer k , i.e. $r_{ij}^* = r_{ij}$. This shows that the equivalence levels of second order equivalence points of R are the corresponding entries of R^* .

By analogies, for any k the equivalence levels of k -th order equivalence points of R are the corresponding entries of R^* .

4'. Obviously, by the methods in Definition 2.5, we can form a similar matrix $R^{<k>}$ by $n \times n$ matrix R finally, and the equivalence points of $R^{<k>}$ form a chain, hence each entries of R^* are all equivalence levels of R , by Proposition 2.6.

This completes our proof.

3. AN ALGORITHM OF FUZZY CLUSTERING

On the basis of the fuzzy similar matrix R given, by the Propositions 2.6 and 2.7, the procedure for direct clustering may be given as the following

I. Write all first order equivalence points (i, j) and the levels r_{ij} of R , denoted by $r_{ij} / (i, j)_1$.

II. Write the equivalence chains of R . If all equivalence points of R form a chain, then turn to IV.

III. Write the maximal elements of set $U_{i,j}$ of intersection points of each equivalence chains. Make matrix $R^{<2>}$. repeat the procedure I, II, until the equivalence points of $R^{<k>}$ form a chain.

IV. Because a k -th order equivalence level $r_{ij}^{<k>}$ is a coefficient of similarity and $r_{ij}^{<k>}$ is an entry of R , then there exist fixed u, v such that $r_{ij}^{<k>} = r_{uv}$, where r_{uv} is the entry of R . Hence, we may write $r_{ij}^{<k>} / (i, j)_k$ as $r_{ij}^{<k>} / (u, v)$ or $r_{uv} / (u, v)$, where $r_{uv} / (u, v)$ express the maximal possibility degree of which the

patterns u and v belong to the same class according to the equivalence relation R^* .

Finally, we make the clustering graph by $\{r_{uv} / (u,v) \mid r_{uv}$ are the equivalence levels of $R, 1 \leq u, v \leq n.\}$

Example:

Let

$$R = \begin{bmatrix} 1 & 0.9 & 0.7 & 0.6 & 0.4 & 0.3 \\ 0.9 & 1 & 0.4 & 0.2 & 0.5 & 0.6 \\ 0.7 & 0.4 & 1 & 0.8 & 0.1 & 0.5 \\ 0.6 & 0.2 & 0.8 & 1 & 0.5 & 0.3 \\ 0.4 & 0.5 & 0.1 & 0.5 & 1 & 0.95 \\ 0.3 & 0.6 & 0.5 & 0.3 & 0.95 & 1 \end{bmatrix}$$

Obviously, R is a similar matrix, not an equivalence matrix.

The first order equivalence points and levels are

$$0.9 / (1,2), 0.8 / (3,4), 0.95 / (5,6)$$

respectively, the equivalence chains $e_1 = \{1,2\}, e_2 = \{3,4\}, e_3 = \{5,6\}$.

Make the matrix $R^{<2>}$.

$$r_{12}^{<2>} = \bigvee_{\substack{i=1,2 \\ j=3,4}} r_{ij} = r_{13} = 0.7, \quad r_{13}^{<2>} = \bigvee_{\substack{i=1,2 \\ j=5,6}} r_{ij} = r_{26} = 0.6, \quad r_{23}^{<2>} = \bigvee_{\substack{i=3,4 \\ j=5,6}} r_{ij} \\ = r_{54} = 0.5, \quad r_{kk}^{<2>} = 1, \quad k=1,2,3.$$

hence

$$R^{<2>} = \begin{bmatrix} 1 & 0.7 & 0.6 \\ 0.7 & 1 & 0.5 \\ 0.6 & 0.5 & 1 \end{bmatrix}$$

The second order equivalence points and levels are $0.7 / (1,2)_2, 0.6 / (3,1)_2$, they form a chain $e = \{1,2,3\}$. Hence, whole entries of R^* are $0.9 / (1,2), 0.8 / (3,4), 0.95 / (5,6), 0.7 / (1,2)_2 = 0.7 / (1,3), 0.6 / (3,1)_2 = 0.6 / (2,6)$, which are illustrated in Fig.1.

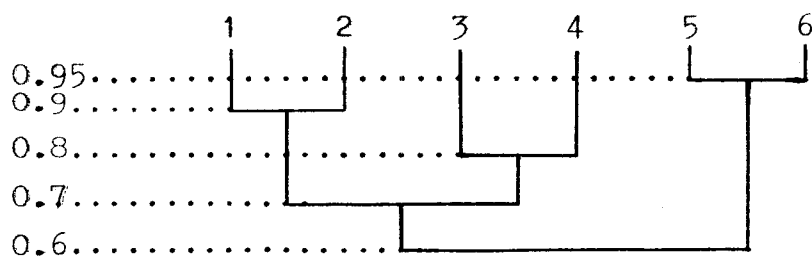


Fig 1. Hierarchical clustering graph.

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