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NOTES AND COMMENTS

NOTE ON ULTRAMETRIC HIERARCHICAL CLUSTERING ALGORITHMS

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Milligan presented the conditions that are required for a hierarchical clustering strategy to be monotonic, based on a formula by Lance and Williams. In the present paper, the statement of the conditions is improved and shown to provide necessary and sufficient conditions.

Key words: monotonic hierarchical clustering strategies.

Milligan [1979] showed:
The hierarchical clustering strategy $(\alpha_1, \alpha_2, \beta, \gamma)$ based on Lance and Williams [1967] formula:

$$d_{k(ij)} = \alpha_1 d_{ki} + \alpha_2 d_{kj} + \beta d_{ij} + \gamma |d_{ki} - d_{kj}| \tag{1}$$

is monotonic, i.e.,

$$\forall d_{ij}, d_{ki}, d_{kj}: d_{k(ij)} \geq d_{ij} \tag{2}$$

if the following conditions hold:

$$\begin{aligned} &\text{(i)} \quad \gamma \geq 0 \vee (\gamma < 0 \wedge |\gamma| \leq \alpha_1, \alpha_2), \\ &\text{(ii)} \quad \min(\alpha_1, \alpha_2) \geq 0, \\ &\text{(iii)} \quad \alpha_1 + \alpha_2 + \beta \geq 1. \end{aligned} \tag{3}$$

In this note we present an improved version of this theorem.
The hierarchical clustering strategy $(\alpha_1, \alpha_2, \beta, \gamma)$ based on Lance and Williams formula (1) is monotonic iff the following conditions hold:

$$\begin{aligned} &\text{(i)} \quad \gamma \geq -\min(\alpha_1, \alpha_2), \\ &\text{(ii)} \quad \alpha_1 + \alpha_2 \geq 0, \\ &\text{(iii)} \quad \alpha_1 + \alpha_2 + \beta \geq 1. \end{aligned} \tag{4}$$

Proof: The conditions (4) are sufficient: (4) ⇒ (2). Without loss of generality [because of the symmetry of i and j in (1)], let:

$$d_{ki} \geq d_{kj}. \tag{5}$$

Therefore:

$$\begin{aligned} d_{k(ij)} &= \alpha_1 d_{ki} + \alpha_2 d_{kj} + \beta d_{ij} + \gamma |d_{ki} - d_{kj}| \\ &= (\alpha_1 + \gamma) d_{ki} + (\alpha_2 - \gamma) d_{kj} + \beta d_{ij}. \end{aligned}$$

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TABLE 1. Examples of solutions (d_{ki}, d_{kj}, d_{ij}), $d_{ki} \geq d_{kj} \geq d_{ij}$ of inequality (7)

CASE		(d_{ki}, d_{kj}, d_{ij})
$\alpha_1 + \gamma < 0$		$d_{ki} \geq \max\left(\frac{(1-\beta)d_{ij} + (\alpha_2 - \gamma)d_{kj}}{\alpha_1 + \gamma}, d_{kj}\right)$
$\alpha_1 + \gamma \geq 0$	$\alpha_1 + \alpha_2 < 0$	$d_{ki} = d_{kj} > \max\left(\frac{1-\beta}{\alpha_1 + \alpha_2}, 1\right)d_{ij}$
	$\alpha_1 + \alpha_2 \geq 0$ $\alpha_1 + \alpha_2 + \beta < 1$	$d_{ki} \geq d_{kj} \geq d_{ij}$

From (4i) it follows $\alpha_1 + \gamma \geq 0$. Combining this with (5) we get:

$$d_{k(ij)} \geq (\alpha_1 + \gamma + \alpha_2 - \gamma)d_{kj} + \beta d_{ij}$$

$$d_{k(ij)} \geq (\alpha_1 + \alpha_2)d_{kj} + \beta d_{ij}.$$

Again, from (4ii) $\alpha_1 + \alpha_2 \geq 0$ and by the nature of the hierarchical clustering procedure that clusters together the two closest objects (clusters) at each step, $d_{kj} \geq d_{ij}$. This gives:

$$d_{k(ij)} \geq (\alpha_1 + \alpha_2 + \beta)d_{ij},$$

and finally from (4iii) we get the desired result:

$$d_{k(ij)} \geq d_{ij}.$$

To prove that the conditions (4) are also necessary is a much longer, but routine, task. The idea of the proof is the following: if the strategy $(\alpha_1, \alpha_2, \beta, \gamma)$ does not fulfill the conditions (4), there exists at least one solution (d_{ki}, d_{kj}, d_{ij}) of the nonmonotonicity inequality:

$$d_{k(ij)} < d_{ij} \tag{6}$$

i.e., there exists a counterexample to monotonicity.

To carry out this idea we assume again that (5) holds. Then we can rewrite (6) as follows:

$$(\alpha_1 + \gamma)d_{ki} + (\alpha_2 - \gamma)d_{kj} < (1 - \beta)d_{ij}. \tag{7}$$

Analyzing (7) we can see that the inequality (6) is solvable in all of the cases represented in the Table 1, which form, under the assumption (5), exactly the complement of the conditions (4).

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