

Paths characteristics in determination of optimal clustering procedure for a data set

No.	Steps in a typical cluster analysis	Path's number										
		1	2	3	4	5	6	7	8	9		
I	Selection of objects and variables	data matrix $[x_{ij}]$										
II	Measurement scale of variables	ratio	ratio	interval or mixed ¹	ordinal ²	multi-state nominal ³	binary	ratio	interval or mixed ¹	ratio	interval or mixed ¹	
	Selection of normalization formula ⁴	n6 – n11	n1 – n5	n1 – n5	N.A.	N.A.		without normalization		n6-n11 / n1-n5	n1-n5	
	Transformed measurement scale of variables	ratio	interval	interval	ordinal	multi-state nominal	binary	ratio	interval or mixed ¹	ratio / interval	interval	
III	Selection of distance measure ⁵	d1 – d7	d1 – d5	d1 – d5	d8	d9	b1 – b10	d1 – d7	d1 – d5	N.A.		
IV	Selection of clustering method ⁶	m1 – m8								m9		
V	Maximal number of possible variants	[(6 x 7 x 5) + (6 x 1 x 3)] + [(5 x 5 x 5) + (5 x 1 x 3)] = 368		(5 x 5 x 5) + (5 x 1 x 3) = 140		1 x 5 = 5	1 x 5 = 5	10 x 5 = 50	(7 x 5) + (1 x 3) = 38	(5 x 5) + (1 x 3) = 28	11	5
	Number of all classifications	$LK = (\text{maxClusterNo} - \text{minClusterNo} + 1) \cdot LW_p$, where minClusterNo minimal number of clusters, maxClusterNo maximal number of clusters, LW_p – number of variants for p -th path.										
	Internal cluster quality index	1. Calinski & Harabasz (G1) ⁷ 2. Baker & Hubert (G2) 3. Hubert & Levin (G3) 4. Silhouette (S) 5. Krzanowski & Lai (KL) ⁷				1. N.A. 2. G2 3. G3 4. S 5. N.A.			1. G1 2. G2 3. G3 4. S 5. KL		1. G1 2. N.A. 3. N.A. 4. N.A. 5. KL	

¹ Ratio & interval.² We can use ratio, interval or mixed data (ratio, interval, ordinal), however these data are treated as ordinal because in the construction of the GDM2 distance measure only such relations as: “equal to”, “higher than”, “lower than” are taken into account.³ We can use ratio, interval, ordinal or mixed data (ratio, interval, ordinal, nominal), however these data are treated as nominal because in the construction of the Sokal & Michener distance measure only such relations as: “equal to”, “not equal to” are taken into account.⁴ n1 – (x-mean)/sd, n2 – (x-Me)/MAD, n3 – (x-mean)/range, n4 – (x-min)/range, n5 – (x-mean)/max[abs(x-mean)], n6 – (x/sd), n7 – (x/range), n8 – (x/max), n9 – (x/mean), n10 – (x/sum), n11 – x/sqrt(SSQ).⁵ d1 – Manhattan, d2 – Euclidean, d3 – Chebychev (max), d4 – squared Euclidean, d5 – GDM1, d6 – Canberra, d7 – Bray-Curtis; d8 – GDM2, d9 – Sokal & Michener; b1 – b10 (available in R dist.binary procedure): b1 = Jaccard; b2 = Sokal & Michener; b3 = Sokal & Sneath (1); b4 = Rogers & Tanimoto; b5 = Czekanowski; b6 = Gower & Legendre (1); b7 = Ochiai; b8 = Sokal & Sneath (2); b9 = Phi of Pearson; b10 = Gower & Legendre (2).⁶ m1 – single link, m2 – complete link, m3 – average link, m4 – McQuitty, m5 – k -medoids (PAM), m6 – ward, m7 – centroid, m8 – median, m9 – k -means. For clustering methods m6–m8 squared Euclidean distance is used only.⁷ with argument `centrotypes="centroids"`.

N.A. – Not Applicable.

Source: Walesiak, M., Dudek, A. (2006), *Symulacyjna optymalizacja wyboru procedury klasyfikacyjnej dla danego typu danych – oprogramowanie komputerowe i wyniki badan*, Prace Naukowe AE we Wroclawiu no. 1126, 120-129.