

replication.Mod(clusterSim)

### Modification of replication analysis for cluster validation

Formally, replicating clusters proceeds as follows (see Breckenridge [2000], 262-263; Milligan [1996], 368-369; Gordon [1999], 184; Walesiak [2007]):

1. The data are randomly divided into two samples: sample  $A$  (arbitrarily primary) and sample  $B$  (replication). Data must exist on the same set of variables in both samples.

2. Sample  $A$  is clustered (via `kmeans`, `pam` or any hierarchical agglomerative method: `single`, `complete`, `average`, `mcquitty`, `median`, `centroid`, `Ward`) into  $u$  clusters  $A = \{A_1, \dots, A_u\}$ . Decisions regarding variable normalization, distance measure, and selection of the number of clusters are to be completed. Once clusters have been identified, the centroids of  $u$  clusters are computed (for metric data) or  $u$  representative objects (often called centrotypes or medoids) are selected (for metric or nonmetric data).

3. Sample  $B$  is clustered, using the same clustering procedure, into  $u$  clusters  $B = \{B_1, \dots, B_u\}$ .

4. Determine the distances between sample  $B$  objects to the centroids (or medoids) of sample  $A$ . Assign objects from sample  $B$  to their nearest centroid (or medoid). Each element in sample  $B$  is assigned to the nearest centroid (or medoid) determined from the sample  $A$  (this provides a partition of sample  $B$  into no more than  $u$  clusters). This produces a clustering of sample  $B$  based on characteristics of sample  $A$ :  $B^* = \{B_1^*, \dots, B_u^*\}$ .

5. Repeat steps 1-4  $S$  times ( $S$  – the number of simulations).

6. Compute a measure of agreement (mean corrected Rand index) between two clusterings  $B$  and  $B^*$  for  $S$  simulations. The level of agreement between the two partitions reflects the stability of the clustering in the data.

### References

- Breckenridge, J.N. (2000), *Validating cluster analysis: consistent replication and symmetry*, "Multivariate Behavioral Research", 35 (2), 261-285.
- Gordon, A.D. (1999), *Classification*, Chapman and Hall/CRC, London.
- Hubert, L., Arabie, P. (1985), *Comparing partitions*, "Journal of Classification", no. 1, 193-218.
- Milligan, G.W. (1996), *Clustering validation: results and implications for applied analyses*, In P. Arabie, L.J. Hubert, G. de Soete (Eds.), *Clustering and classification*, World Scientific, Singapore, 341-375.
- Walesiak, M. (2007), *Ocena stabilnosci wyników klasyfikacji z wykorzystaniem analizy replikacji*, Prace Naukowe AE we Wrocławiu (in preparation).