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Crisp cluster validity indices: Dunn, Davies-Bouldin and Silhouette

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At the beginning of this article, I appreciate the scholar ***Joaquim Viegas*** *from the University of Lisbo in Portugal, sincerely. It is because of his article that I have solved some problems about Dunn index. Thanks for your work!*

I. Definition

Adapted from Arbelaitz et al. (2003) [1].

Dataset $\boldsymbol{X}$ of N objects (samples) represented as objects (samples) in a p-dimensional space:

$$\boldsymbol{X} = [\overrightarrow{x_1}, \overrightarrow{x_2}, \ldots, \overrightarrow{x_N}]^\top = [\overrightarrow{\text{sample}_1}, \overrightarrow{\text{sample}_2}, \ldots, \overrightarrow{\text{sample}_N}]^\top \subseteq \mathfrak{R}^p$$

$$\forall i \in \{1, 2, \ldots, N\} \hookrightarrow \overrightarrow{x_i} = [a_{i1}, a_{i2}, \ldots, a_{ip}]$$

A partition or clustering in $\boldsymbol{X}$ is a set of disjoint clusters that partition $\boldsymbol{X}$ into K groups:

$$\mathbb{C} = \{C_1, C_2, \ldots, C_K\} \quad \text{where} \quad \forall k \neq j \hookrightarrow \bigcup_{C_k \in \mathbb{C}} C_k = \boldsymbol{X},\ C_k \cap C_j = \varnothing$$

The centroid of a cluster C_k is its mean vector:

$$\overline{C_k} = \frac{\sum\limits_{x_i \in C_k} x_i}{|C_k|}$$

Dataset mean vector:

$$\overline{\boldsymbol{X}} = \frac{\sum\limits_{x_i \in \boldsymbol{X}} x_i}{N}$$

Euclidean distance:

$$d(x_i, x_k) = \sqrt{\sum_{j=1}^{p} (x_{ij} - x_{kj})}$$

II. Davies-Bouldin Index (DBI↓) [2]

It estimates the cohesion based on the distance from the points in a cluster to its centroid and the separation based on the distance between centroids. It is defined as:

$$\text{DBI}(\mathbb{C}) = \frac{1}{K} \sum_{C_k \in \mathbb{C}} \max_{C_j \in \mathbb{C} \setminus C_k} \left\{ \frac{\frac{1}{|C_k|} \sum\limits_{x_i \in C_k} d(x_i, \overline{C_k}) + \frac{1}{|C_j|} \sum\limits_{x_i \in C_j} d(x_i, \overline{C_j})}{d(\overline{C_k}, \overline{C_j})} \right\}$$

III. Dunn Index (DI↑) [3]

It is a ratio-type index where the cohesion is estimated by the nearest neighbor distance and the separation by the maximum cluster diameter. The original index is defined as:

$$\mathrm{DI}(\mathbb{C}) = \frac{\min\limits_{C_k \in \mathbb{C}} \left\{ \min\limits_{C_j \in \mathbb{C} \setminus C_k} \left[\min\limits_{x_i \in C_k} \min\limits_{x_j \in C_j} \{ d(x_i, x_j) \} \right] \right\}}{\max\limits_{C_k \in \mathbb{C}} \left\{ \max\limits_{x_i, x_j \in C_k} [d(x_i, x_j)] \right\}}$$

$$\text{where} \quad \min_{x_i \in C_k} \min_{x_j \in C_j} \{ d(x_i, x_j) \} = \min_{x_i \in C_k; x_j \in C_j} \{ d(x_i, x_j) \}$$

IV. Silhouette Index (Sil↑) [4]

This index is a normalized summation-type index. The cohesion is measured based on the distance between all the points in the same cluster and the separation is based on the nearest neighbor distance. It is defined as:

$$\mathrm{Sil}(\mathbb{C}) = \frac{1}{N} \sum_{C_k \in \mathbb{C}} \sum_{x_i \in C_k} \frac{\min\limits_{C_j \in \mathbb{C} \setminus C_k} \left[\frac{1}{|C_j|} \sum\limits_{x_j \in C_j} d(x_i, x_j) \right] - \frac{1}{|C_k|} \sum\limits_{x_j \in C_k} d(x_i, x_j)}{\max \left\{ \frac{1}{|C_k|} \sum\limits_{x_j \in C_k} d(x_i, x_j), \min\limits_{C_j \in \mathbb{C} \setminus C_k} \left[\frac{1}{|C_j|} \sum\limits_{x_j \in C_j} d(x_i, x_j) \right] \right\}}$$

$$\text{where} \quad \sum_{C_k \in \mathbb{C}} \sum_{x_i \in C_k} \Longleftrightarrow \sum_{C_k \in \mathbb{C}; x_i \in C_k}$$

References

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[4] Peter Rousseeuw. Silhouettes: A graphical aid to the interpretation and validation of cluster analysis. *Journal of Computational and Applied Mathematics*, 20:53-65, November 1987. sil cvi.