A Novel Idea of The Validation Criterion of Clustering

Kou AMANO[†‡§]
amano@brc.riken.jp

[†] RIKEN
[‡] University of Tsukuba
[§] National Institute of Agrobiological Sciences

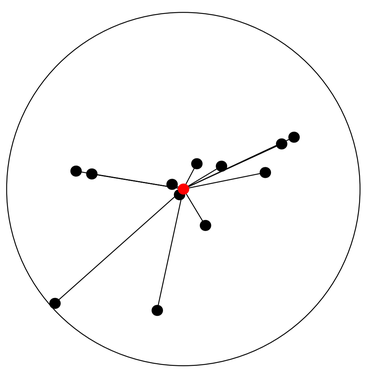
Introduction

This paper introduce a new index of cluster validity only based on simplisity of cluster structure.

- Non-hierarchical clustering is the task of the k-partition problems with heuristics,
- and the solutions are neither global nor unique,
- hence it needs indices to assess the clustering results.

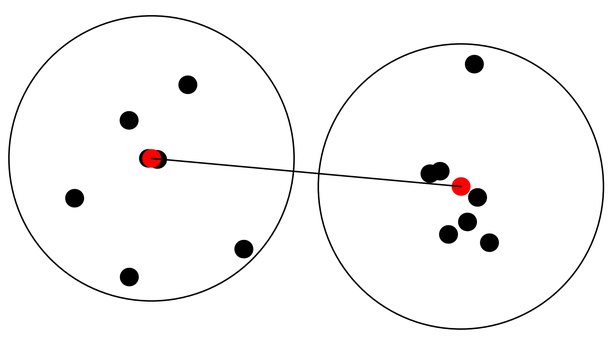
Existing indices

- Criteria
  - Compactness



Within-cluster distance

  - Separability

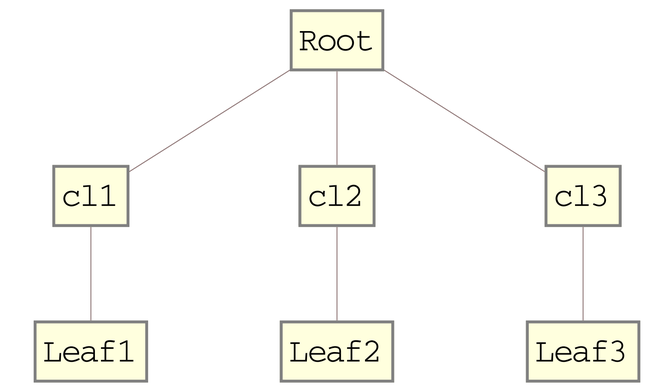


Between-cluster distance

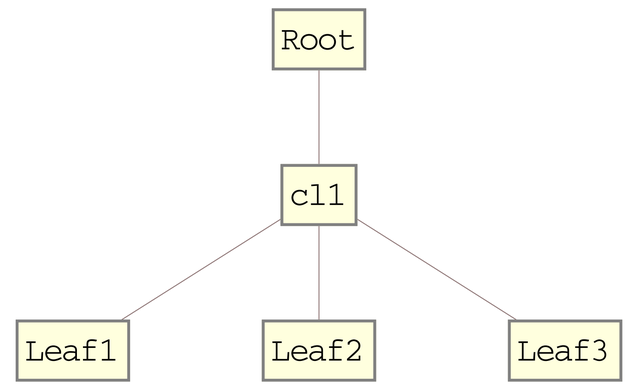
- Elements
  - Number of clusters
  - Number of members of each cluster
  - representative (or each) distance within cluster
  - representative (or each) distance between clusters
- Well-known indices
  - Dunn index[1]
  - Calinski-Harabazs index[2]
  - Davies-Bouldin index[3]

Desirable properties of indices

- The index would indicate identical values to cluster structures with the same topology:



$k = N\ ;\ \{\{Leaf1\},\{Leaf2\},\{Leaf3\}\} \overset{simplify}{\longrightarrow} \{Leaf1, Leaf2, Leaf3\}$

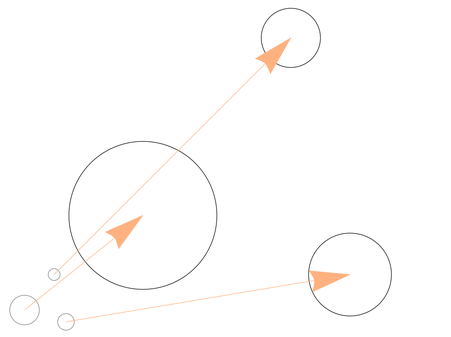


$k = 1\ ;\ \{\{Leaf1, Leaf2, Leaf3\}\} \overset{simplify}{\longrightarrow} \{Leaf1, Leaf2, Leaf3\}$

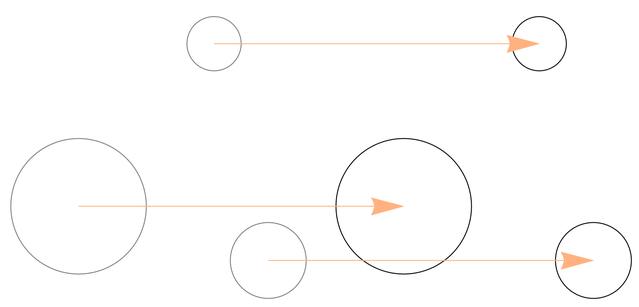
$\downarrow$

$Id_{k=N}(\boldsymbol{S}) = Id_{k=1}(\boldsymbol{S})$

- The index would indicate identical values to sample sets with a similar distribution:



Scale ; $Id(a \times \boldsymbol{S}) = Id(\boldsymbol{S})$



Shift ; $Id(\boldsymbol{b} + \boldsymbol{S}) = Id(\boldsymbol{S})$

Simplicity Index(SI): a novel index

- New criterion
  - Simplisity
- Elements
  - k : number of clusters
  - c : number of members of each cluster
  - v : space capacity
- Definition

$$SI = k \prod_{n=1}^{k} c_n^{\frac{r_n}{R}}$$

where r_n : radius of cluster n, and R : radius of complete samples. $\frac{r_n}{R}$ is used for v.

Simplicity Ratio(SR): a derivative of SI

- Definition

$$SR = SI/N$$

where N : total number of samples.

- Failure detection

$$\begin{cases} SR < 1 & Success \\ SR \geq 1 & Failure \end{cases}$$

Conclusion

The index SI and the derivative SR have been introduced. These are only based on simplisity of the cluster structure.

References and Acknowledgement

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[Ack] Dr. Kaoru Fukami, RIKEN BioResource Center
[Ack] Mr. Masamichi Wada, JST
[Ack] Mathematica Kenkyu-Kai

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