The Area under the ROC Curve as a Criterion for Clustering Evaluation

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based on the data only, such as the average intra-cluster distance

Internal criteria

e.g., Silhouette Index, Davies-Bouldin Index, Dunn Index

Advantages/disadvantages:

- Do not need to have the true class label.
- Biased towards one clustering algorithm.

External criteria

e.g., Rand Statistics, Jaccard Coefficient, Fowlkes and Mallows Index

Advantages/disadvantages:

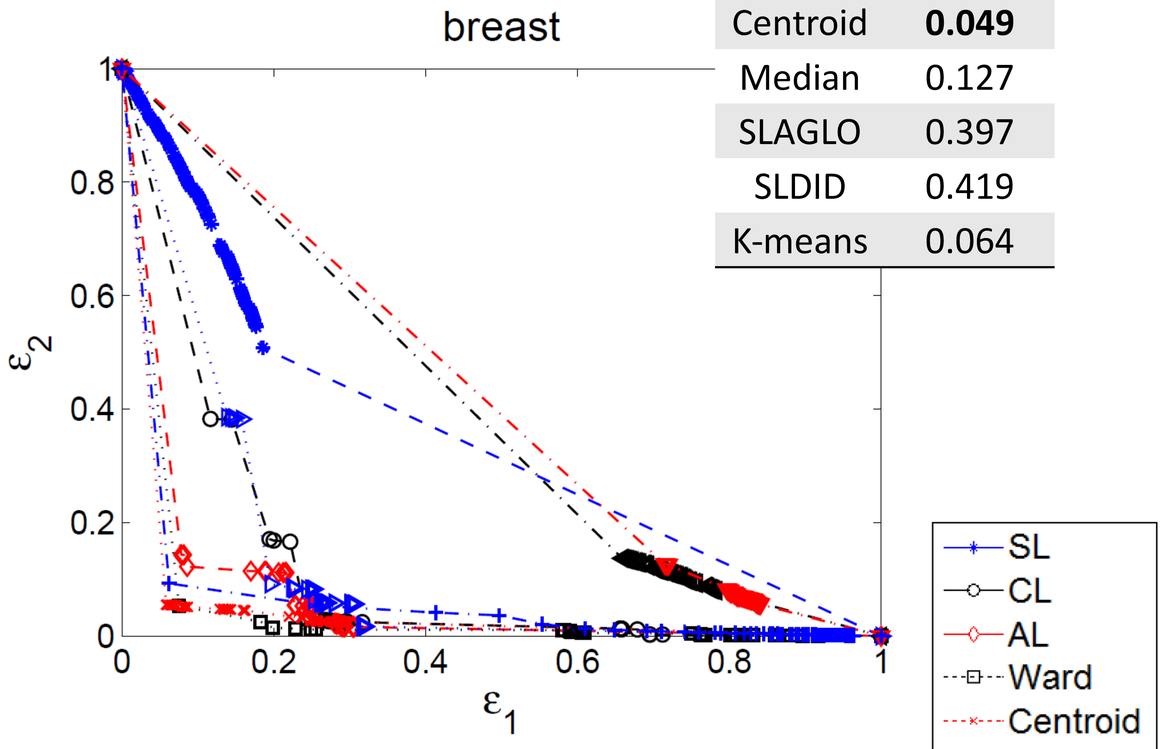
- Need to have the true class label for each object.

Designed for a fixed number of clusters

ROC curve and **AUC**
(to study the robustness of clustering algorithms for several number of clusters, *k*)

ROC curve and AUC when we have access to all labeling information

	AUC
SL	0.351
CL	0.121
AL	0.070
Ward	**0.049**
Centroid	**0.049**
Median	0.127
SLAGLO	0.397
SLDID	0.419
K-means	0.064



Consider two given points $\mathbf{x}_a$, $\mathbf{x}_b$.

➢ Type I error:

$$\varepsilon_1 \equiv P(\mathbf{x}_a \in C_i, \mathbf{x}_b \in C_j | \mathbf{x}_a, \mathbf{x}_b \in P_l), i \neq j$$

➢ Type II error:

$$\varepsilon_2 \equiv P(\mathbf{x}_a, \mathbf{x}_b \in C_i | \mathbf{x}_a \in P_j, \mathbf{x}_b \in P_l), j \neq l$$

➢ A clustering partition *C* is **concordant** with the true labeling, *P*, of the data if

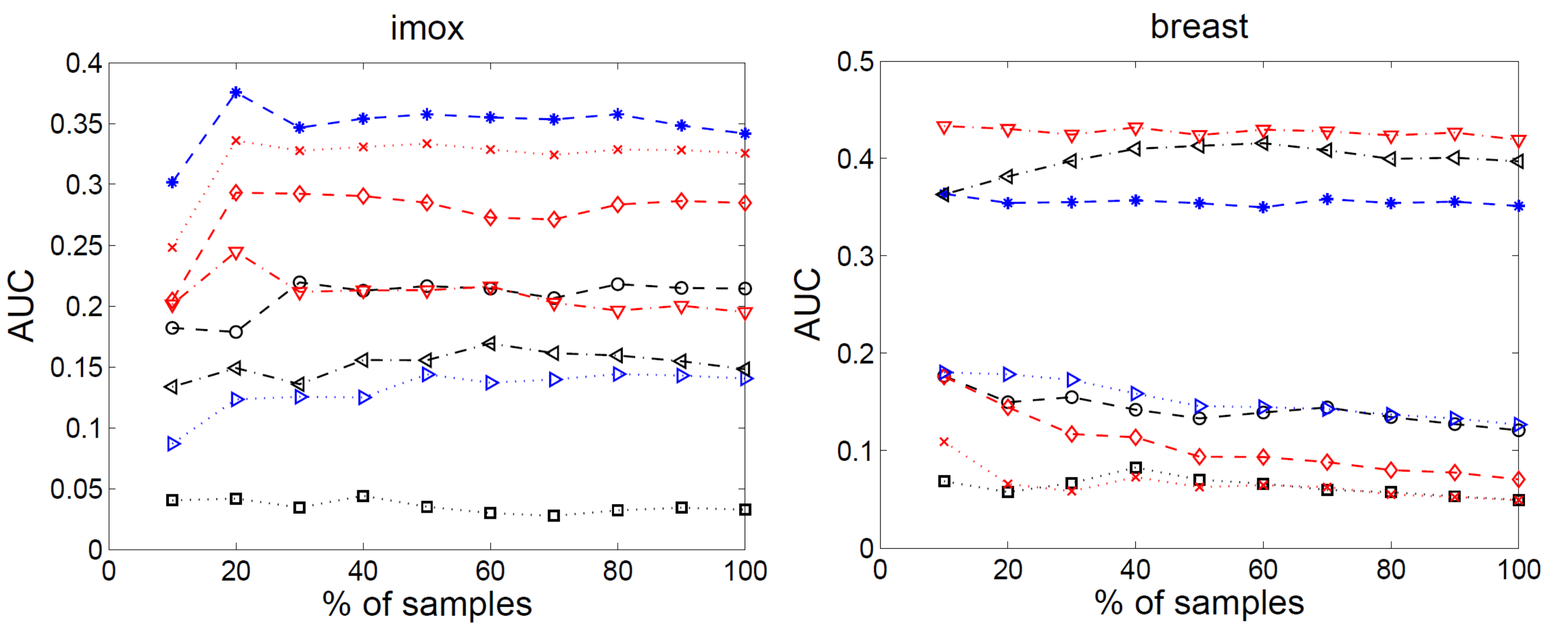
$$\begin{cases} \varepsilon_1 = 0 & \text{if } k \leq m \\ \varepsilon_2 = 0 & \text{if } k \geq m \\ \varepsilon_1 = \varepsilon_2 = 0 & \text{if } k = m. \end{cases}$$

➢ A ROC curve is **proper** if, when varying *k*, ε_1 increases whenever ε_2 decreases and vice-versa.

➢ Evaluate Robustness: A clustering algorithm is more **robust** to the choice of *k* than another algorithm if the former's AUC is smaller than the latter's.

Semi-supervised Context

We might have only labels for a small part of the entire dataset.



Conclusions

➢ In the literature, external and internal criteria are designed to **evaluate clustering** algorithms for a **fixed number of clusters**.

➢ The proposed measure quantifies the performance of an algorithm for **several *k* simultaneously**.

- This allows measuring how robust a clustering algorithm is to the choice of *k*.

➢ In the semi-supervised context, the whole dataset is used to perform clustering, whereas the AUC is computed with only a part of the data.

➢ The measure proposed can be used to automatically detect whether the currently labeled data is already enough.

➢ Allow us to extrapolate classes from the labeled data to the unlabeled data, if one can find a clustering algorithm which yields low and consistent AUC value for the labeled portion.

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