UNIVERSITAT DE BARCELONA

Course. Introduction to Machine Learning

Work 1. Clustering Exercise

Session 3

Course 2021-2022

Dr. Maria Salamó Llorente

Dept. Mathematics and Informatics,

Faculty of Mathematics and Informatics,

University of Barcelona

Contents

1. Introduction (session 1)
2. Preprocess the data (session 1)
3. OPTICS with sklearn (session 2)
4. K-Means (your own code) (session 2)
5. K-Modes, K-Medoids or K-Prototypes (your own code) (session 2)
6. Fuzzy clustering (your own code) (session 3)
7. Validation techniques (using sklearn validation metrics) (session 3)

Fuzzy Clustering

Fuzzy Clustering

- Data points are given partial **degree of membership** in multiple nearby clusters
- Central point in the fuzzy clustering is always no unique partitioning of the data in a collection of clusters
- In this membership value is assigned to each cluster. Sometimes this membership has been used to decide whether the data points belong to the cluster or not

Fuzzy C-Means Clustering (FCM)

- Several approximations
  - **FCM**: Fuzzy C-Means Clustering (Bezdek, 1981)
  - **PCM**: Possibililistic C-Means Clustering (Krishnapuram - Keller, 1993)
  - **FPCM**: Fuzzy Possibililistic C-Means (N. Pal - K. Pal - Bezdek, 1997)

- The most well-known fuzzy clustering algorithm is FCM
- Bezdek introduced the idea of a fuzzification parameter (m) in the range [1, n]
  - When m = 1 the effect is a crisp clustering of points
  - When m >1 the degree of fuzziness among points i the decision space increases

Fuzzy C-Means Clustering

Iterative FCM algorithm

- Guess Initial Cluster Centers $V_0 = \left(V_{1,0}, \ldots, V_{c,0}\right) \in \mathcal{R}^{cp}$
- Alternating Optimization (AO)

```
t ← 0
REPEAT
   t ← t +1
   Compute matrix U_t   (Eq.1)
   Compute associated clusters centers V_t (Eq.2)
UNTIL ( t = T   or ‖ V_t − V_{t−1} ‖≤ ε )
```

$(U,V) \leftarrow (U_t,V_t)$

References of Fuzzy Clustering

- *C. Bezdek (1981): "Pattern Recognition with Fuzzy Objective Function Algoritms", Plenum Press, New York*
- **J. C. Bezdek, R. Ehrlich, W. Full (1984). FCM: The fuzzy C-Means Algorithm.**
- James C. Bezdek, James Keller, Raghu Krishnapuram and Nikhil R. Pal (1999), *Fuzzy Models and Algorithms for Pattern Recognition and Image Processing*, Kluwer Academic Publishers, TA 1650.F89.
- R. Krishnapuram and J. M. Keller (1993) A possibilistic approach to clustering," *IEEE Transactions on Fuzzy Systems*, Vol. 1, No. 2, pp. 98-110.
- N. R. Pal, K. Pal and J. C. Bezdek (1997), "A mixed c-means clustering model," *Proceedings of the Sixth IEEE International Conference on Fuzzy Systems*, Vol. 1, pp. 11-21.
- Jun Yan, Michael Ryan and James Power, *Using fuzzy logic Towards intelligent systems*, Prentice Hall, 1994.

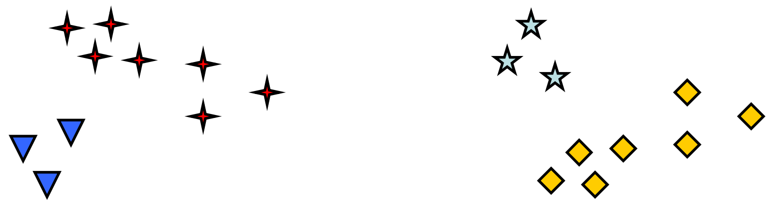
Validation of clustering

Clustering Validation

How many clusters?

Six Clusters

Two Clusters



Four Clusters

Which is the best clustering?

Cluster validation

Supervised classification:

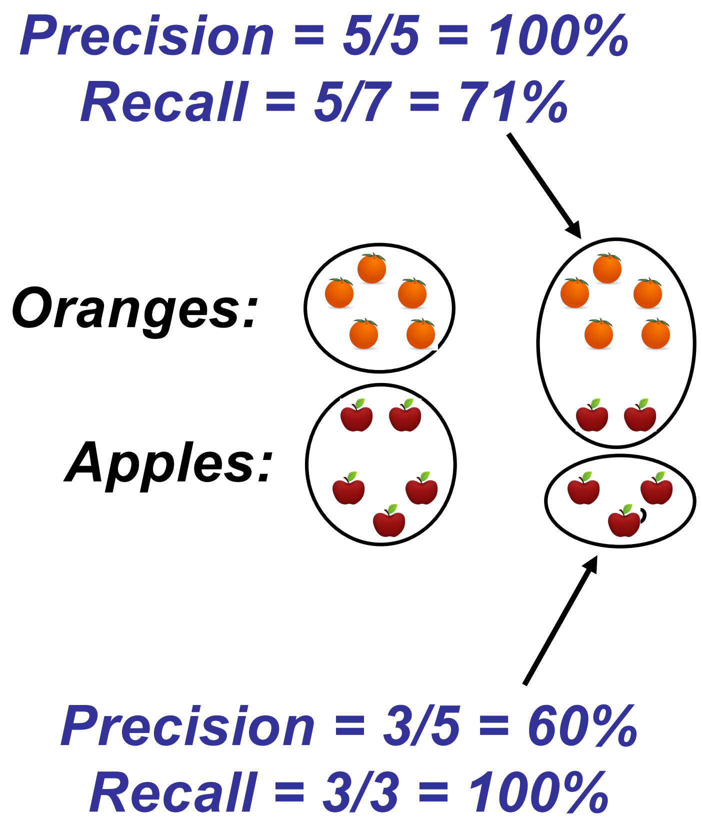
- Class labels known for ground truth
- Accuracy, precision, recall

Cluster analysis

- No class labels

Validation need to:

- Compare clustering algorithms
- Solve number of clusters
- Avoid finding patterns in noise



What Is A Good Clustering?

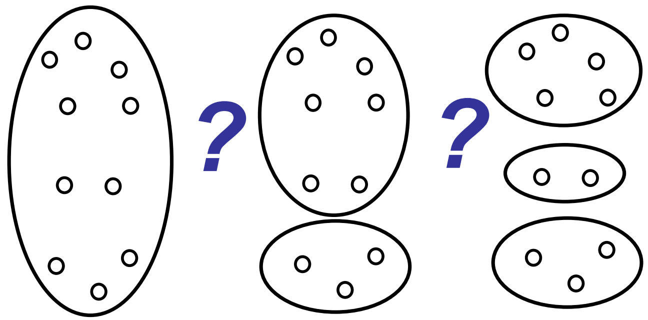
- **Internal criterion**: A good clustering will produce high quality clusters in which:
  - the intra-class (that is, intra-cluster) similarity is high
  - the inter-class similarity is low
  - The measured quality of a clustering depends on both the example representation and the similarity measure used
- **External criterion**: The quality of a clustering is also measured by its ability to discover some or all of the hidden patterns or latent classes
  - Assessable with gold standard data

UNIVERSITAT DE BARCELONA

Measuring clustering validity

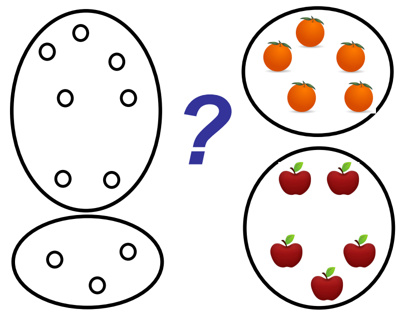
Internal Index

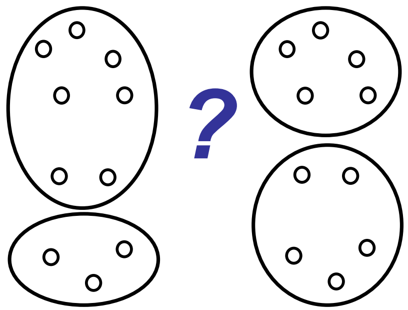
- Validate *without* external info
- With different number of clusters
- Solve the number of clusters



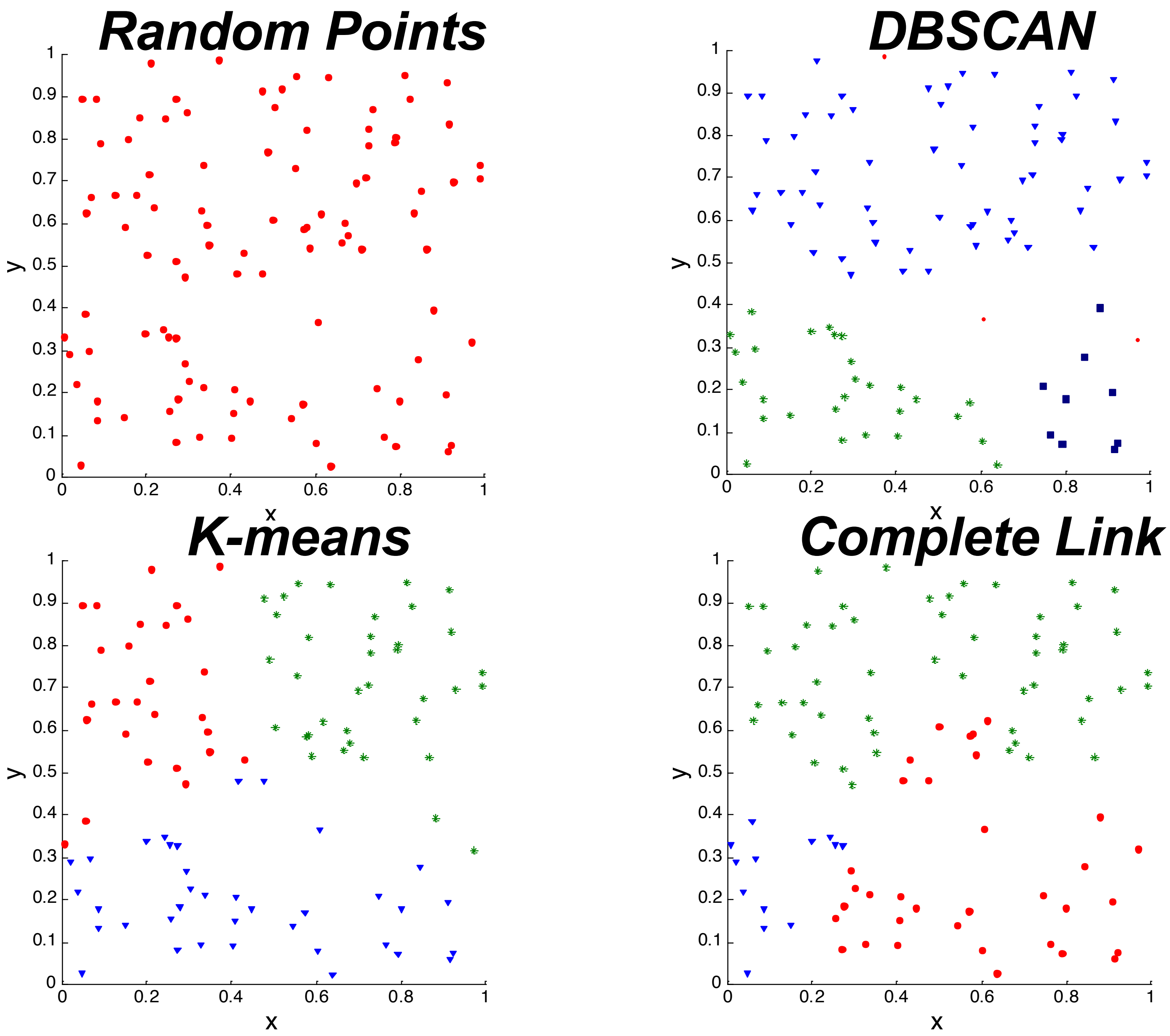
External Index

- Validate against ground truth
- Compare two clusters: (how similar)



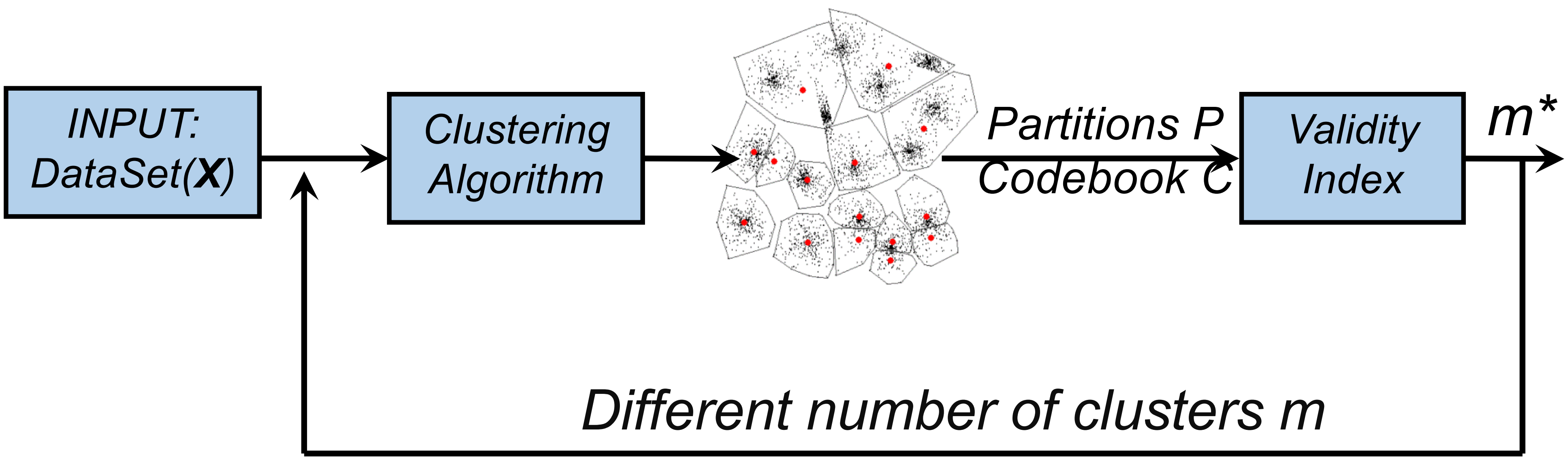


Clustering of random data



Cluster validation process

- **Cluster validation** refers to procedures that evaluate the results of clustering in a **quantitative** and **objective** fashion [Jain & Dubes, 1988]
  - How to be "quantitative": To employ the measures.
  - How to be "objective": To validate the measures!



Internal indexes

- Ground truth is rarely available but unsupervised validation must be done.
- Minimizes (or maximizes) internal index:
  - Variances of within cluster and between clusters
  - Rate-distortion method
  - F-ratio
  - Davies-Bouldin index (DBI)
  - Bayesian Information Criterion (BIC)
  - Silhouette Coefficient
  - Minimum description principle (MDL)
  - Stochastic complexity (SC)

Internal indexes

Table B.1: Formulas for internal indexes

Name	Formula
SSW	$SSW = \frac{1}{N} \sum_{i=1}^{N} \left\| x_i - C_{p_i} \right\|^2$
SSB	$SSB = \frac{2}{M(M-1)} \sum_{i=1}^{M} \sum_{j=1, j \neq i}^{M} \left\| C_i - C_j \right\|^2$
Calinski-Harabasz index	$CH = \frac{SSB/(M-1)}{SSW(N-M)}$
Hartigan	$H_M = (\frac{SSW_M}{SSW_{M+1}} - 1)(N - M - 1)$ $or : H_M = \log (SSB_M / SSW_M)$
Krzanowski-Lai index	$diff_M = (M-1)^{2/D} SSW_{M-1} - M^{2/D} SSW_M$ $KL_M = \lvert diff_M \rvert \, / \, \lvert diff_{M+1} \rvert$
Ball&Hall	$BH_M = SSW_M / M$
Xu-index	$Xu = D \log (\sqrt{SSW_M / (DN^2)}) + \log M$
Dunn's index	$Dunn = \sum_{i=1}^{M} \frac{\max (\left\| x_j - C_i \right\|^2)_{j \in C_i}}{}$
Davies&Bouldin index	$R_{ij} = \frac{S_i + S_j}{d_{ij}}, i \neq j$ $where : d_{ij} = \left\| C_i - C_j \right\|^2, S_i = \frac{1}{n_i} \sum_{j=1}^{n_i} \left\| x_j - C_i \right\|^2$ $and, R_i = \max_{j=1,\ldots,M} R_{ij}, i = 1, \ldots, M$ $DBI = \frac{1}{M} \sum_{i=1}^{M} R_i$

Internal indexes

Silhouette Coefficients	$a(x_i) = \frac{1}{n_m - 1} \sum_{j=1, j\neq i}^{n_m} \lVert x_i - x_j \rVert^2_{x_i, x_j \in C_m}$ $b(x_i) = \min_t \{ \frac{1}{n_t} \sum_{j \in C_t} \lVert x_i - x_j \rVert^2 \}_{x_i \notin C_t}$ $s(x_i) = \frac{b(x_i) - a(x_i)}{\max(a(x_i), b(x_i))}$ $SC = \frac{1}{N} \sum_{i=1}^{N} s(x_i)$ $b(x_i) = \min \{ \sum_{t \neq m} \lVert C_t - C_m \rVert^2 \}_{x_i \notin C_t} (SC'2008)$
RMSSTD	$RMSSTD = \frac{\sum_{\substack{k=1,\dots,M \\ d=1,\dots,D}} \sum_{i=1}^{n_{kd}} (x_i - \overline{x^d})^2}{\sum_{\substack{k=1,\dots,M \\ d=1,\dots,D}} (n_{kd} - 1)}$
R-square	$RS = \frac{SST - SSW}{SST} = \frac{\sum_{d=1,\dots,D} \sum_{i=1}^{n_d} (x_i - \overline{x^d})^2 - \sum_{\substack{k=1,\dots,M \\ d=1,\dots,D}} \sum_{i=1}^{n_{kd}} (x_i - \overline{x^d})^2}{\sum_{d=1,\dots,D} \sum_{i=1}^{n_d} (x_i - \overline{x^d})^2}$
Bayesian Information Criterion	$BIC = L * N - \frac{1}{2} M(D+1) \sum_{i=1}^{M} \log(n_i)$
Xie-Beni	$XB = \frac{\sum_{i=1}^{N} \sum_{k=1}^{M} u_{ik}^2 \lVert x_i - C_k \rVert^2}{N \min_{t \neq s} \{ \lVert C_t - C_s \rVert^2 \}}$
Partition Coefficient	$PC = \sum_{i=1}^{N} \sum_{k=1}^{M} u_{ik}^2 / N$
Partition Entropy	$PE = -(\sum_{i=1}^{N} \sum_{k=1}^{M} u_{ik} \log(u_{ik}))/N$

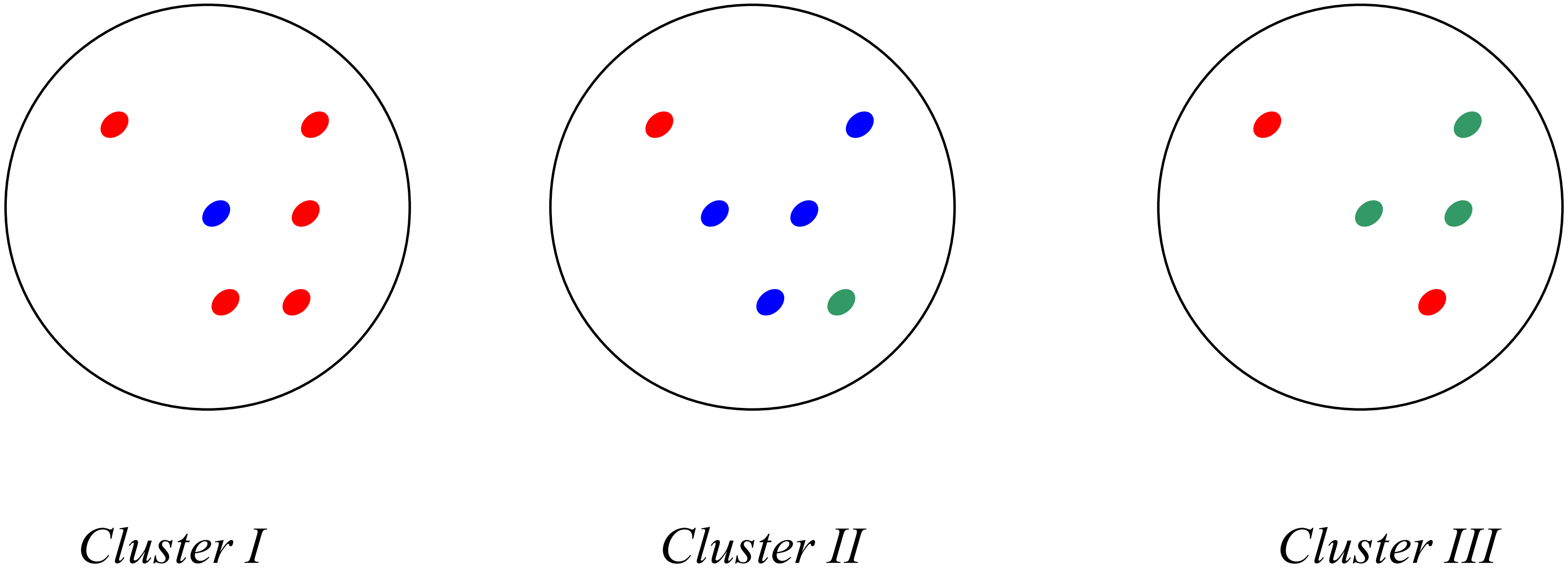
Soft partitions

External Indexing

- Assesses clustering with respect to ground truth
- Assume that there are C gold standard classes, while our clustering algorithms produce *k* clusters, $\pi_1, \pi_2, \ldots, \pi_k$ with n_i members.
- **Simple measure**: purity, the ratio between the dominant class in the cluster π_i and the size of cluster π_i

$$Purity(\pi_i) = \frac{1}{n_i} \max_j (n_{ij}) \quad j \in C$$

Purity Example



Cluster I: Purity = 1/6 (max(5, 1, 0)) = 5/6 (0,83)

Cluster II: Purity = 1/6 (max(1, 4, 1)) = 4/6 (0,66)

Cluster III: Purity = 1/5 (max(2, 0, 3)) = 3/5 (0,60)

Pair-counting measures

Measure the number of pairs that are in:

Same class **both** in *P* and *G*.

$$a = \frac{1}{2}\sum_{i=1}^{K}\sum_{j=1}^{K'} n_{ij}(n_{ij}-1)$$

Same class in *P* but different in *G*.

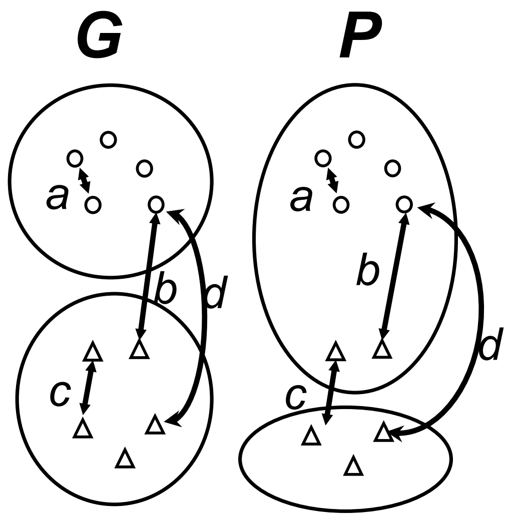
$$b = \frac{1}{2}\left(\sum_{j=1}^{K'} n_{.j}^2 - \sum_{i=1}^{K}\sum_{j=1}^{K'} n_{ij}^2\right)$$

Different classes in *P* but same in *G*.

$$c = \frac{1}{2}\left(\sum_{i=1}^{K} n_{i.}^2 - \sum_{i=1}^{K}\sum_{j=1}^{K'} n_{ij}^2\right)$$

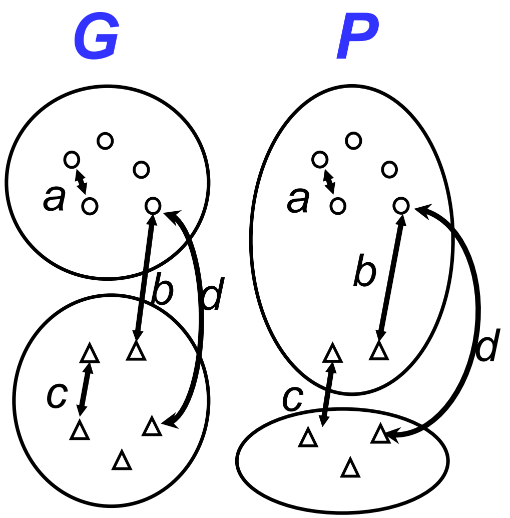
Different classes **both** in *P* and *G*.

$$d = \frac{1}{2}\left(N^2 + \sum_{i=1}^{K}\sum_{j=1}^{K'} n_{ij}^2 - \left(\sum_{i=1}^{K} n_{i.}^2 + \sum_{j=1}^{K'} n_{.j}^2\right)\right)$$



Rand and Adjusted Rand index

[Rand, 1971] [Hubert and Arabie, 1985]



Agreement: *a, d*
Disagreement: *b, c*

$$RI(P,G) = \frac{a+d}{a+b+c+d}$$

$$ARI = \frac{RI - E(RI)}{1 - E(RI)}$$

External indexes

If true class labels (*ground truth*) are known, the validity of a clustering can be verified by comparing the class labels and clustering labels.

$$
\begin{array}{c|c}
N & \cdot \\
\hline
\cdot & n_{\cdot\cdot}
\end{array}
=
\begin{array}{cccc|c}
n_{11} & n_{12} & \cdots & n_{1l} & n_{1\cdot} \\
n_{21} & n_{22} & \cdots & n_{2l} & n_{2\cdot} \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
n_{k1} & n_{k2} & \cdots & n_{kl} & n_{k\cdot} \\
\hline
n_{\cdot 1} & n_{\cdot 2} & \cdots & n_{\cdot l} & n_{\cdot\cdot}
\end{array}
$$

n_{ij} = number of objects in class i and cluster j

External indexes

- Pair counting
  - Chi-Squared Coefficient
  - Rand Index
  - Adjusted Rand Index
  - Fowlkes-Mallows Index
  - Mirkin Metric
- Other measures
  - Information theoretic
    - Mutual Information Metric (MI), Normalized Mutual Information, Variation of Information
  - Set matching
    - Jaccard Index, Normalized Van Dongen, Pair Set Index

Summary of external indexes

Table 1: External Cluster Validation Measures.

	Measure	Notation	Definition	Range
1	Entropy	E	$-\sum_i p_i(\sum_j \frac{p_{ij}}{p_i} \log \frac{p_{ij}}{p_i})$	$[0, \log K']$
2	Purity	P	$\sum_i p_i(\max_j \frac{p_{ij}}{p_i})$	(0,1]
3	F-measure	F	$\sum_j p_j \max_i [2\frac{p_{ij}}{p_i}\frac{p_{ij}}{p_j}/(\frac{p_{ij}}{p_i}+\frac{p_{ij}}{p_j})]$	(0,1]
4	Variation of Information	VI	$-\sum_i p_i \log p_i - \sum_j p_j \log p_j - 2\sum_i \sum_j p_{ij} \log \frac{p_{ij}}{p_i p_j}$	$[0, 2\log \max(K, K')]$
5	Mutual Information	MI	$\sum_i \sum_j p_{ij} \log \frac{p_{ij}}{p_i p_j}$	$(0, \log K']$
6	Rand statistic	R	$[\binom{n}{2} - \sum_i \binom{n_{i\cdot}}{2} - \sum_j \binom{n_{\cdot j}}{2} + 2\sum_{ij}\binom{n_{ij}}{2}]/\binom{n}{2}$	(0,1]
7	Jaccard coefficient	J	$\sum_{ij}\binom{n_{ij}}{2}/[\sum_i \binom{n_{i\cdot}}{2} + \sum_j \binom{n_{\cdot j}}{2} - \sum_{ij}\binom{n_{ij}}{2}]$	[0,1]
8	Fowlkes and Mallows index	FM	$\sum_{ij}\binom{n_{ij}}{2}/\sqrt{\sum_i \binom{n_{i\cdot}}{2}\sum_j \binom{n_{\cdot j}}{2}}$	[0,1]
9	Hubert Γ statistic I	Γ	$\frac{\binom{n}{2}\sum_{ij}\binom{n_{ij}}{2} - \sum_i \binom{n_{i\cdot}}{2}\sum_j \binom{n_{\cdot j}}{2}}{\sqrt{\sum_i \binom{n_{i\cdot}}{2}\sum_j \binom{n_{\cdot j}}{2}[\binom{n}{2} - \sum_i \binom{n_{i\cdot}}{2}][\binom{n}{2} - \sum_j \binom{n_{\cdot j}}{2}]}}$	(-1,1]
10	Hubert Γ statistic II	Γ'	$[\binom{n}{2} - 2\sum_i \binom{n_{i\cdot}}{2} - 2\sum_j \binom{n_{\cdot j}}{2} + 4\sum_{ij}\binom{n_{ij}}{2}]/\binom{n}{2}$	[0,1]
11	Minkowski score	MS	$\sqrt{\sum_i \binom{n_{i\cdot}}{2} + \sum_j \binom{n_{\cdot j}}{2} - 2\sum_{ij}\binom{n_{ij}}{2}}/\sqrt{\sum_j \binom{n_{\cdot j}}{2}}$	$[0, +\infty)$
12	classification error	ε	$1 - \frac{1}{n}\max_\sigma \sum_j n_{\sigma(j),j}$	[0,1)
13	van Dongen criterion	VD	$(2n - \sum_i \max_j n_{ij} - \sum_j \max_i n_{ij})/2n$	[0, 1)
14	micro-average precision	MAP	$\sum_i p_i(\max_j \frac{p_{ij}}{p_i})$	(0,1]
15	Goodman-Kruskal coefficient	GK	$\sum_i p_i(1 - \max_j \frac{p_{ij}}{p_i})$	[0,1)
16	Mirkin metric	M	$\sum_i n_{i\cdot}^2 + \sum_j n_{\cdot j}^2 - 2\sum_i \sum_j n_{ij}^2$	$[0, 2\binom{n}{2})$

Note: $p_{ij} = n_{ij}/n$, $p_i = n_{i\cdot}/n$, $p_j = n_{\cdot j}/n$.

Clustering evaluation in Python

- Clustering performance evaluation

```
from sklearn import metrics
```

  - Adjusted Rand index
  - Mutual information based scores
  - Homogeneity, completeness and V-measure
  - Fowlkes-Mallows scores
  - Silhouette Coefficient
  - Calinski-Harabaz Index
  - Davies-Bouldin Index
  - Contingency Matrix

References on cluster validation

1. G.W. Milligan, and M.C. Cooper, “An examination of procedures for determining the number of clusters in a data set”, *Psychometrika*, Vol.50, 1985, pp. 159-179.
2. E. Dimitriadou, S. Dolnicar, and A. Weingassel, “An examination of indexes for determining the number of clusters in binary data sets”, *Psychometrika*, Vol.67, No.1, 2002, pp. 137-160.
3. D.L. Davies and D.W. Bouldin, "A cluster separation measure “, *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 1(2), 224-227, 1979.
4. J.C. Bezdek and N.R. Pal, "Some new indexes of cluster validity “, *IEEE Transactions on Systems, Man and Cybernetics*, 28(3), 302-315, 1998.
5. H. Bischof, A. Leonardis, and A. Selb, "MDL Principle for robust vector quantization“, *Pattern Analysis and Applications*, 2(1), 59-72, 1999.
6. P. Fränti, M. Xu and I. Kärkkäinen, "Classification of binary vectors by using DeltaSC-distance to minimize stochastic complexity", *Pattern Recognition Letters*, 24 (1-3), 65-73, January 2003.

References on cluster validation

7. G.M. James, C.A. Sugar, "Finding the Number of Clusters in a Dataset: An Information-Theoretic Approach". *Journal of the American Statistical Association*, vol. 98, 397-408, 2003.
8. P.K. Ito, Robustness of ANOVA and MANOVA Test Procedures. In: Krishnaiah P. R. (ed), *Handbook of Statistics 1: Analysis of Variance*. North-Holland Publishing Company, 1980.
9. I. Kärkkäinen and P. Fränti, "Dynamic local search for clustering with unknown number of clusters", *Int. Conf. on Pattern Recognition (ICPR'02*), Québec, Canada, vol. 2, 240-243, August 2002.
10. D. Pellag and A. Moore, "X-means: Extending K-Means with Efficient Estimation of the Number of Clusters", *Int. Conf. on Machine Learning* (ICML), 727-734, San Francisco, 2000.
11. S. Salvador and P. Chan, "Determining the Number of Clusters/Segments in Hierarchical Clustering/Segmentation Algorithms", *IEEE Int. Con. Tools with Artificial Intelligence* (ICTAI), 576-584, Boca Raton, Florida, November, 2004.
12. M. Gyllenberg, T. Koski and M. Verlaan, "Classification of binary vectors by stochastic complexity ". *Journal of Multivariate Analysis*, 63(1), 47-72, 1997.

References on cluster validation

13. M. Gyllenberg, T. Koski and M. Verlaan, "Classification of binary vectors by stochastic complexity ". *Journal of Multivariate Analysis*, 63(1), 47-72, 1997.
14. X. Hu and L. Xu, "A Comparative Study of Several Cluster Number Selection Criteria", *Int. Conf. Intelligent Data Engineering and Automated Learning* (IDEAL), 195-202, Hong Kong, 2003.
15. Kaufman, L. and P. Rousseeuw, 1990. Finding Groups in Data: An Introduction to Cluster Analysis. *John Wiley and Sons, London*. ISBN: 10:0471878766.
16. [1.3] M.Halkidi, Y.Batistakis and M.Vazirgiannis: Cluster validity methods: part 1, SIGMOD Rec., Vol.31, No.2, pp.40-45, 2002
17. R. Tibshirani, G. Walther, T. Hastie. Estimating the number of clusters in a data set via the gap statistic. *J.R.Statist. Soc. B*(2001) 63, Part 2, pp.411-423.
18. T. Lange, V. Roth, M, Braun and J. M. Buhmann. Stability-based validation of clustering solutions. *Neural Computation*. Vol. 16, pp. 1299-1323. 2004.

UNIVERSITAT DE BARCELONA

References on cluster validation

19. Q. Zhao, M. Xu and P. Fränti, "Sum-of-squares based clustering validity index and significance analysis", *Int. Conf. on Adaptive and Natural Computing Algorithms (ICANNGA'09*), Kuopio, Finland, LNCS 5495, 313-322, April 2009.
20. Q. Zhao, M. Xu and P. Fränti, "Knee point detection on bayesian information criterion", *IEEE Int. Conf. Tools with Artificial Intelligence (ICTAI)*, Dayton, Ohio, USA, 431-438, November 2008.
21. W.M. Rand, "Objective criteria for the evaluation of clustering methods," *Journal of the American Statistical Association*, 66, 846–850, 1971
22. L. Hubert and P. Arabie, "Comparing partitions", *Journal of Classification*, 2(1), 193-218, 1985.
23. P. Fränti, M. Rezaei and Q. Zhao, "Centroid index: Cluster level similarity measure", Pattern Recognition, 2014. (<u>accepted</u>)

Course. Introduction to Machine Learning

Work 1. Clustering Exercise

Session 3

Course 2021-2022

Dr. Maria Salamó Llorente

Dept. Mathematics and Informatics,

Faculty of Mathematics and Informatics,

University of Barcelona