Course. Introduction to Machine Learning

Work 1. Clustering Exercise

Session 3

Course 2023-2024

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Contents

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*
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Validation of clustering

Clustering Validation

How many clusters?

Six Clusters

Two Clusters

Four Clusters

Which is the best clustering?

Cluster validation

Supervised classification:

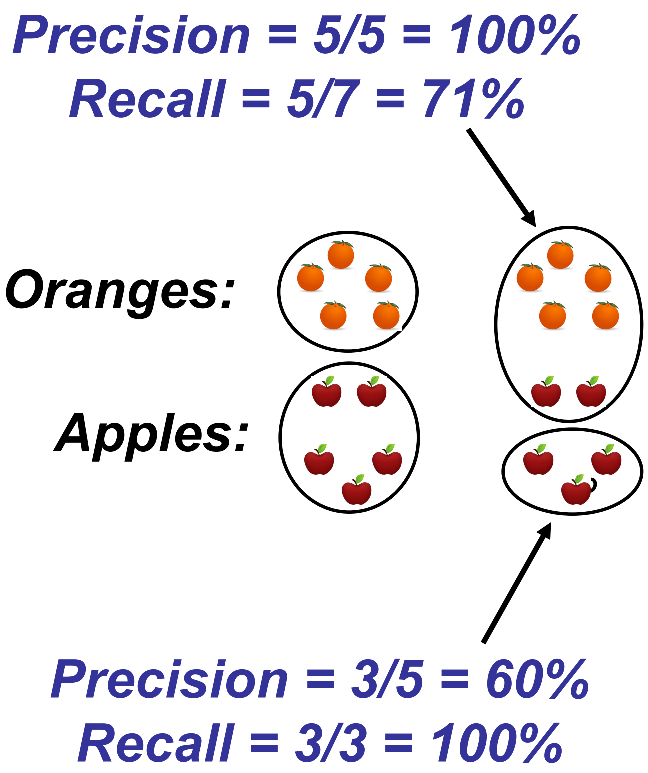
- Class labels known for ground truth
- Accuracy, precision, recall

Cluster analysis

- No class labels

Validation need to:

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



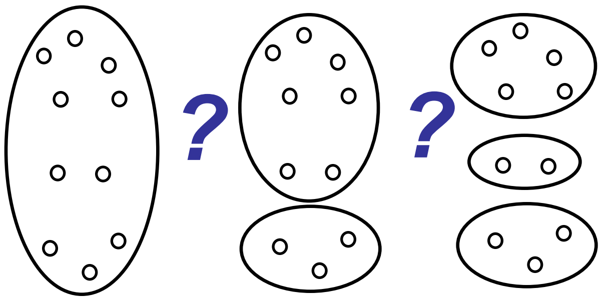
What Is A Good Clustering?

- **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

Measuring clustering validity

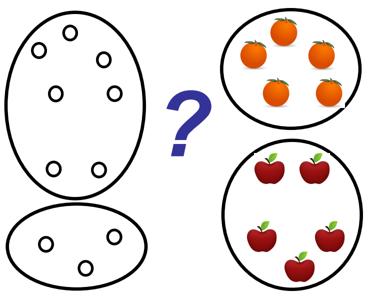
Internal Index

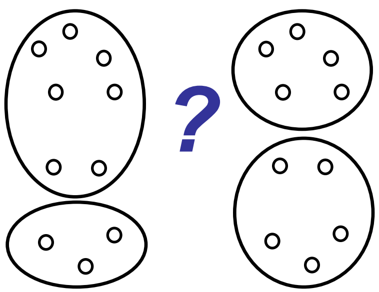
- Validate *without* external info
- With different number of clusters
- Solve the number of clusters



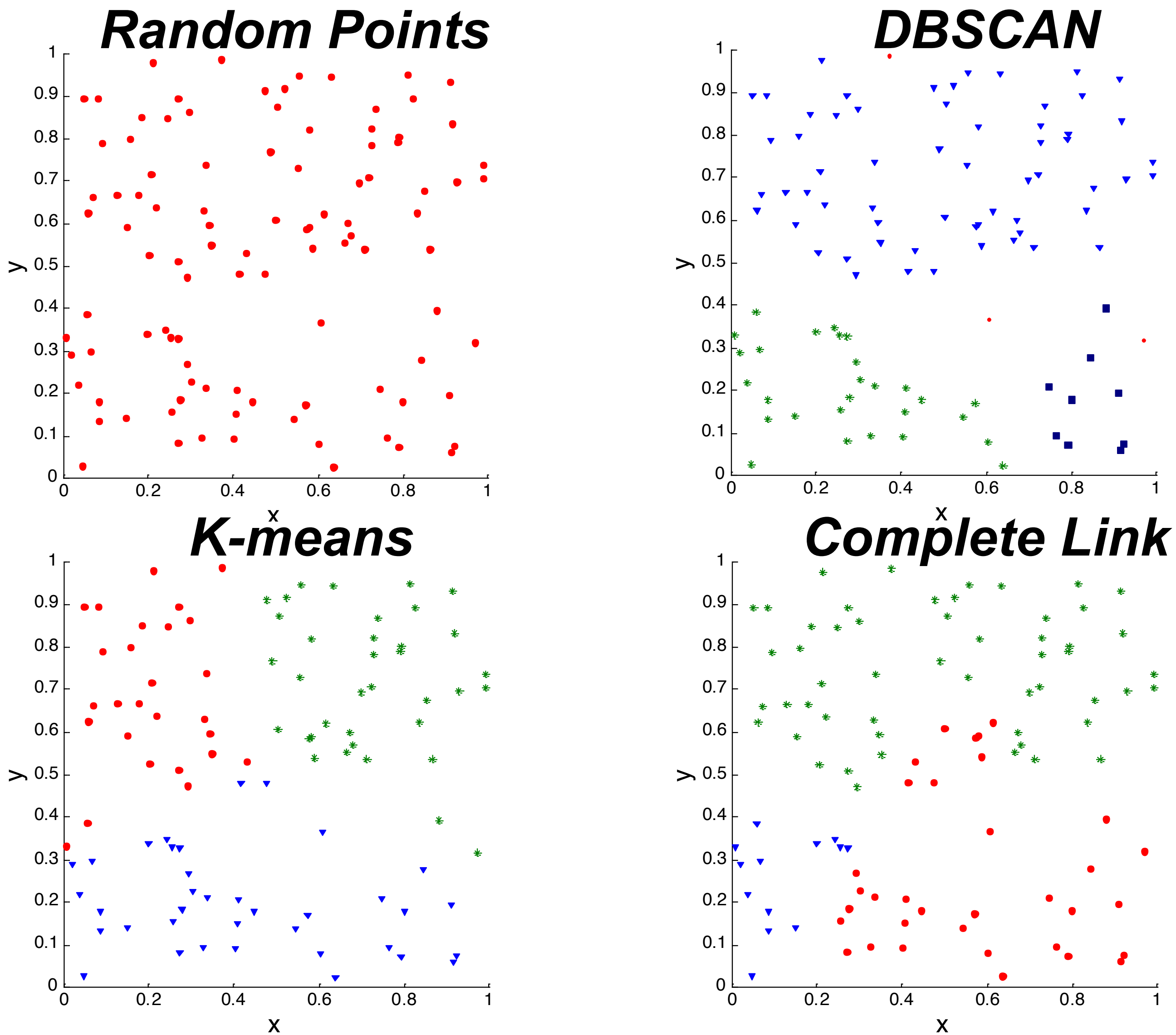
External Index

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



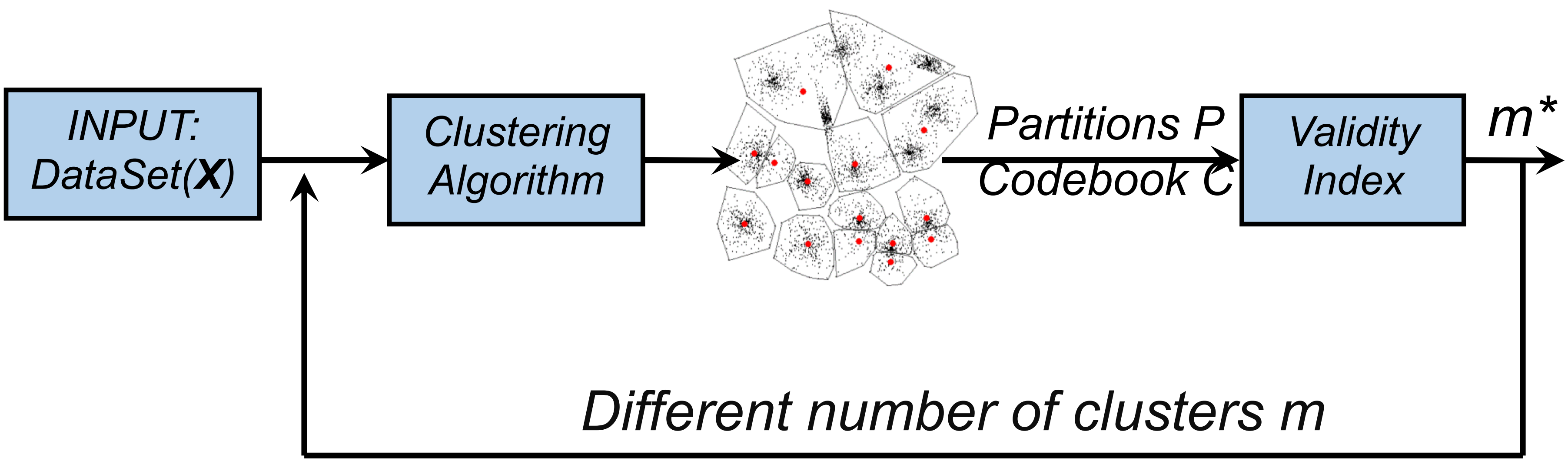


Clustering of random data



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)

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Internal indexes

Table B.1: Formulas for internal indexes

Name	Formula
SSW	$SSW = \frac{1}{N}\sum_{i=1}^{N} \left\Vert x_i - C_{p_i} \right\Vert^2$
SSB	$SSB = \frac{2}{M(M-1)} \sum_{i=1}^{M} \sum_{j=1, j \neq i}^{M} \left\Vert C_i - C_j \right\Vert^2$
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	$Dunn = \sum_{i=1}^{M} \frac{\max(\left\Vert x_j - C_i \right\Vert^2)_{j \in C_i}}{}$
Davies&Bouldin index	$R_{ij} = \frac{S_i + S_j}{d_{ij}}, i \neq j$ $where: d_{ij} = \left\Vert C_i - C_j \right\Vert^2, S_i = \frac{1}{n_i} \sum_{j=1}^{n_i} \left\Vert x_j - C_i \right\Vert^2$ $and, R_i = \max_{j=1,\ldots,M} R_{ij}, i = 1, \ldots, M$ $DBI = \frac{1}{M} \sum_{i=1}^{M} R_i$

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	$RMSSTD = \frac{\sum_{\substack{k=1,\ldots,M \\ d=1,\ldots,D}} \sum_{i=1}^{n_{kd}} (x_i - \overline{x^d})^2}{\sum_{\substack{k=1,\ldots,M \\ d=1,\ldots,D}} (n_{kd} - 1)}$
R-square	$RS = \frac{SST - SSW}{SST} = \frac{\sum_{d \; 1,\ldots,D} \sum_{i=1}^{n_d} (x_i - \overline{x^d})^2 - \sum_{\substack{k=1,\ldots,M \\ d=1,\ldots,D}} \sum_{i=1}^{n_{kd}} (x_i - \overline{x^d})^2}{\sum_{d=1,\ldots,D} \sum_{i-1}^{n_d} (x_i - \overline{x^d})^2}$
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	$PE = -(\sum_{i=1}^{N} \sum_{k=1}^{M} u_{ik} \log(u_{ik})) / N$

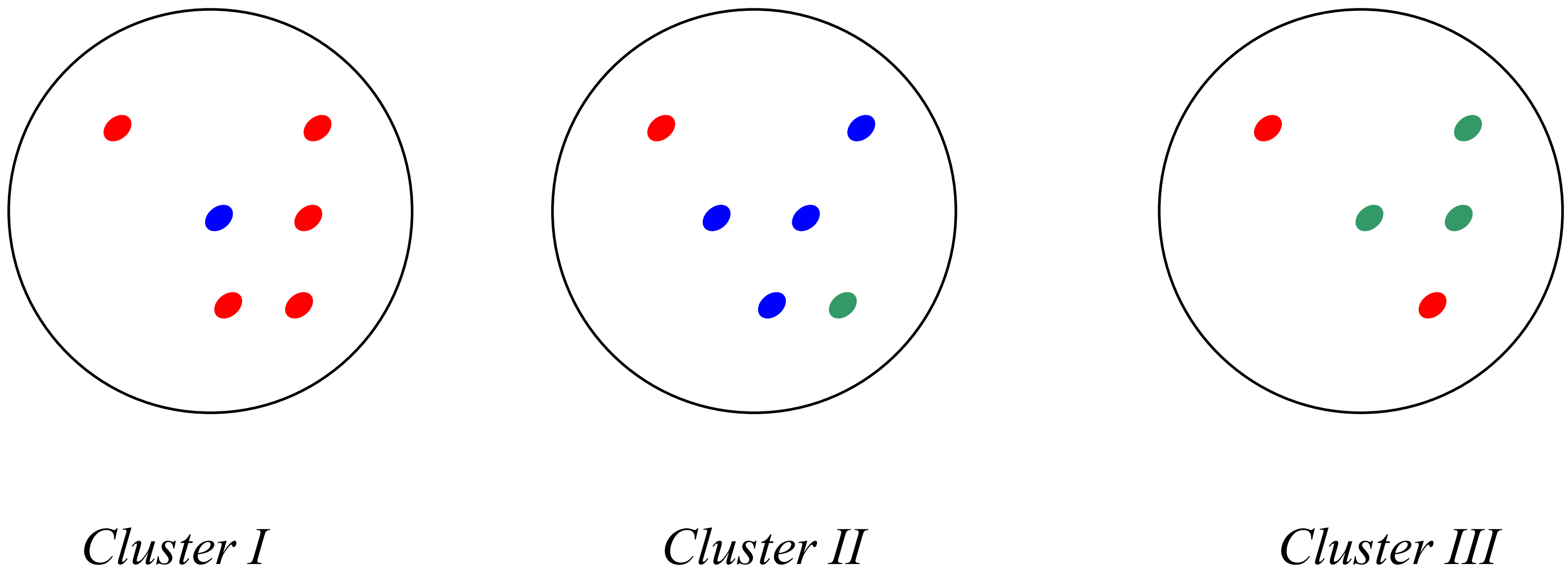
Soft partitions

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*.

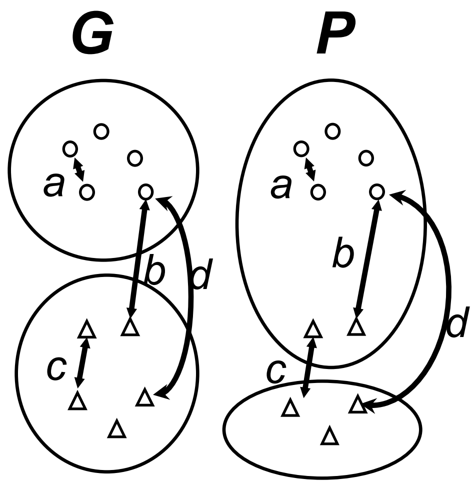
$$b = \frac{1}{2}\left(\sum_{j=1}^{K'} n_{.j}^2 - \sum_{i=1}^{K}\sum_{j=1}^{K'} n_{ij}^2\right)$$

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

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

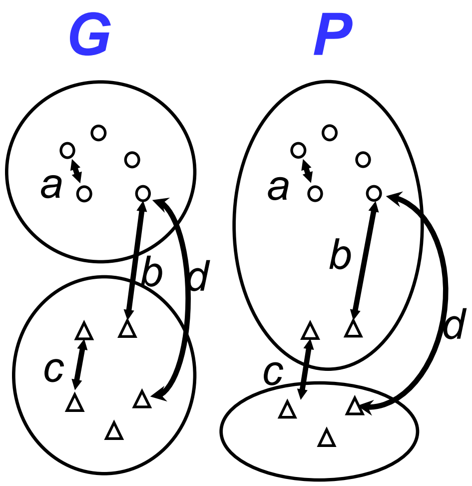
Different classes **both** in *P* and *G*.

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



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.

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

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

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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

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