Clustering Analysis-II

Man-Kwan Shan
Dept. of Computer Science
National Cheng-Chi Univ.

Types of Input Dataset in Clustering Analysis

Types of Input Dataset in Cluster Analysis

- Relational data
- Transactional data
- Sequence
- Time series
- Spatial data
- Mobility Data (maps)
- Textual data
- Tree
- Graph, Social Network
- Image, Video
- Audio, Music

Clustering of Relation Data

- Two different types of data
 - data matrix (two-mode matrix)
 - object-by-attributes structure
 - n objects with p attributes
 - *n* by *p* matrix
 - dissimilarity matrix(one-mode matrix)
 - object-by-object structure
 - a collection of proximity for all pairs of n objects
 - *n* by *n* matrix

Data Matrix (two-mode motrix)

Object ID	ID	Weight	Height	Gender	Birthday	Age
1	111755001	45	165	F	1975/06/06	47
2	111755029	60	170	М	1982/08/30	40
3	111755009	48	160	F	1982/10/29	40
4	111755098	66	180	M	1995/03/16	27
5	111655034	63	175	M	1990/01/15	32

Dissimilarity Matrix (me-mode motiva)

		1	2	3	4	5			
	1	0	2.3	3.4	1.2	3.7			
2	2.3	0	2.0	1.8	2.2				
3	3.4	2.0	0	4.2	0.7				
4	1.2	1.8	4.2	0	4.4				
5	3.7	2.2	0.7	4.4	0				

Input Data Type of Clustering Algorithm

• K-means 2 m-de

partition - Loved

- Single-Link, Complete-Link, Average-Link
- BIRCH 2 mode
- Chameleon | mode
- DBScan | Make
- GMM 2 mde

model -based

hierarchical

情境

- Case 1
 - Clustering program: two mode
 - Data: one mode
 - Can not transform one mode into two mode
- Case 2
 - Clustering program: one mode
 - Data: two mode
 - Transform two mode into one mode based on similarity or distance

Attribute Type of Relational Data

Types of Attributes (variables, features)

- Interval-scaled variables: weight, height 有大具体
 Ordinal: freshman, sophomore, junior, senior 建设
- Ratio-scaled variables 有信成关係但非垛性
- Binary variables: male, female

Interval-scaled Variables

- Interval-scaled variable:
 - continuous measurement of a roughly linear scale
 e.g.: weight, height, temperature
- Measurement unit may affect clustering analysis
 - smaller units → larger range
 e.g. height=1.7 m, weight=60 Kg
 height=170 cm, weight=60 Kg
 - Normalization to [0,1]
 - Min-max normalization: $x' = \frac{x min_A}{max_A min_A}$
 - Z-score normalization: $x' = \frac{x mean_A}{std_A}$

Interval-scaled Variables(cont.)

- Distance between object i, j of p interval attributes
 - Euclidean distance (L2)

$$d(i,j) = \sqrt{|x_{i1} - x_{j1}|^2 + |x_{i2} - x_{j2}|^2 + \dots + |x_{ip} - x_{jp}|^2}$$

- Manhattan (city block) distance (L1)

$$d(i,j) = |x_{i1} - x_{j1}| + |x_{i2} - x_{j2}| + \dots + |x_{ip} - x_{jp}|$$

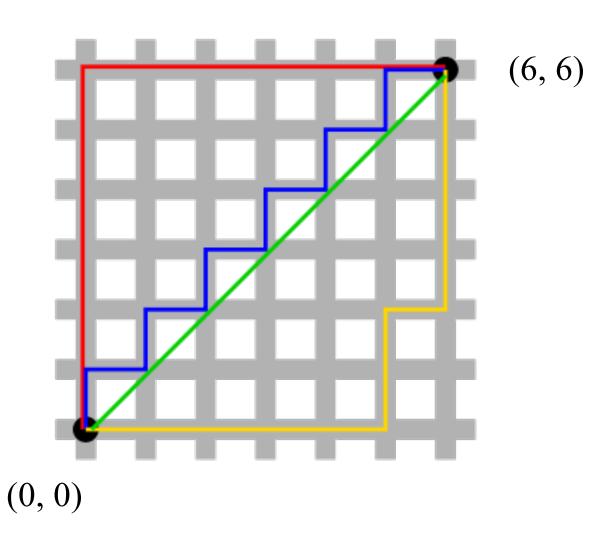
Minkowski distance

$$d(i,j) = \sqrt[q]{|x_{i1} - x_{j1}|^q + |x_{i2} - x_{j2}|^q + \dots + |x_{ip} - x_{jp}|^q}$$

Weighted Manhattan distance

$$d(i,j) = \sqrt[q]{w_1 |x_{i1} - x_{j1}|^q + w_2 |x_{i2} - x_{j2}|^q + \dots + w_p |x_{ip} - x_{jp}|^q}$$

Manhattan (city block) distance



Ordinal Variables

- Ordinal variables
 - relative ordering
 - e.g. assistant, associate, full professor
 - can be obtained by splitting value range of intervalscaled variable into a finite no. of classes
 - distance between objects i, j
 - step 1: replace by corresponding rank
 - step 2: normalize onto [0,1]
 - computed using interval scaled distance

Ratio-scaled Variables

- Ratio-scaled variable
 - positive measurement on a nonlinear scale
 - e.g. Richter scale : as measured with the amplitude of the seismic waves to an arbitrary, minor amplitude.
 - Earthquake that registers 5.0 on the Richter scale has a shaking amplitude 10 times that of an earthquake that registered 4.0
 - e.g. decibel (dB) in acoustics
- Approaches for distance between objects i, j
 - 1. treat like interval-scaled variables
 - 2. apply transformation and treat as interval value
 - 3. treat as continuous ordinal variable

Binary Variables

- Binary variable
 - symmetric
 - -e.g. male, female
 - asymmetric
 - -e.g. HIV positive, HIV negative

Distance between Binary Vectors (cont.)

Example: patient record

Nam	e Gender	fever	cough	Test1	Test2	Test3	Test4
Jack	M	Y	N	P	N	N	N
Mary	y F	Y	N	P	N	P	N
Jim	M	Y	P	N	N	N	N
:	•	:	•	•	:	•	•

gender: symmetric, others: asymmetric

Similarity Between Binary Vectors

- To compute the similarity between two objects, p and q, having only binary attributes.
 - Compute similarities using the following quantities M_{01} = number of attributes where p was 0 and q was 1 M_{10} = number of attributes where p was 1 and q was 0 M_{00} = number of attributes where p was 0 and q was 0 M_{11} = number of attributes where p was 1 and q was 1

Simple Matching

SMC = number of matches / number of attributes $= (M_{11} + M_{00}) / (M_{01} + M_{10} + M_{11} + M_{00}) + insignificant$ Jaccard Coefficients $\int_{0}^{\infty} t de = M_{00} \quad \text{anny from numerator } k \text{ denominator}$

J = number of non-zero-matches / number of not-both-zero attributes

$$= M_{11}/(M_{01} + M_{10} + M_{11}) = \frac{|P \cap Q|}{|P \cup Q|}$$

SMC versus Jaccard: Example

```
p = 0100001001 {b, g, j}

q = 1000001000 {a, g}

a b c d e f g h i j
```

 $M_{01} = 1$ (number of attributes where i was 0 and j was 1)

 $M_{10} = 2$ (number of attributes where i was 1 and j was 0)

 $M_{00} = 6$ (number of attributes where i was 0 and j was 0)

 $M_{11} = 1$ (number of attributes where i was 1 and j was 1)

SMC =
$$(M_{11} + M_{00})/(M_{01} + M_{10} + M_{00} + M_{11})$$

= $(1+6)/(1+2+6+1) = 0.7$
Mos dilutes the numerator & denoninator!

$$J = (M_{11})/(M_{01} + M_{10} + M_{11}) = 1/(1+2+1) = 0.25$$

$$= \frac{|P \cap Q|}{|P \cup Q|}$$

Cosine Similarity

• If d_1 and d_2 are two document vectors, then

$$cos(d_1, d_2) = \frac{d_1 \cdot d_2}{\|d_1\| \|d_2\|},$$

where

 \bullet indicates vector dot product and ||d|| is the length of vector d.

• Example:
$$d_1 = 3205000200$$
 $d_2 = 1000000102$ 1

$$d_1 \bullet d_2 = 3*1 + 2*0 + 0*0 + 5*0 + 0*0 + 0*0 + 0*0 + 2*1 + 0*0 + 0*2 = 5$$

$$||d_1|| = (3*3 + 2*2 + 0*0 + 5*5 + 0*0 + 0*0 + 0*0 + 2*2 + 0*0 + 0*0)^{0.5} = (42)^{0.5} = 6.481$$

$$||d_2|| = (1*1 + 0*0 + 0*0 + 0*0 + 0*0 + 0*0 + 0*0 + 1*1 + 0*0 + 2*2)^{0.5} = (6)^{0.5} = 2.245$$

$$\cos(d_1, d_2) = .3150$$

Distance Between Binary Vectors

- distance between objects i, j
 - symmetric
 - -e.g. male, female
 - $-(M_{01}+M_{10})/(M_{01}+M_{10}+M_{11}+M_{00})$
 - · asymmetric (presence) is more important than 0 (alsence)
 - -e.g. HIV positive, HIV negative
 - $-(M_{01}+M_{10})/(M_{01}+M_{10}+M_{11})$

Distance between Binary Vectors (cont.)

Example: patient record

Name	Gender	fever	cough	Test1	Test2	Test3	Test4
Jack	M	Y	N	P	N	N	N
Mary	F	Y	N	P	N	P	N
Jim	M	Y	P	N	N	N	N
•	:	:	•	•	•	•	•
-							

- gender: symmetric, others: asymmetric
- let Y, P = 1, N=0

$$d(Jack, Mary) = 0 + 1/2 + 0 + 1 = 0.33$$

$$d(Jack, Jim) = 1 + 1/1 + 1 + 1 = 0.67$$

$$d(Jim, Mary) = 1 + 2/1 + 1 + 2 = 0.75$$

Jack 101000 Mary 101010

Jack 101000 Jim 110000

Jim 110000 Mary 101010

Nominal Variables

- Nominal variable
 - generalization of binary variable, take on more than two states
 - e.g. color
 - distance between objects i, j

$$d(i,j) = \frac{p-m}{p} = \frac{\text{#(unmatched variables)}}{\text{*(variables)}}$$

where *p* : #(variables), *m* : #(matched variables)

- can be encoded by asymmetric binary variables
 - e.g. color variable C (R, G, B) => color variables R, G, B

Common Properties of a Distance

- Distances, such as the Euclidean distance, have some well known properties.
 - 1. $d(i, j) \ge 0$ for all i & j and d(i, j) = 0 only if i = j. (Positive definiteness)
 - 2. d(i, j) = d(j, i) for all i and j. (Symmetry)
 - 3. $d(i, k) \le d(i, j) + d(j, k)$ for all i, j, and k. (Triangle Inequality)
 - where d(i, j) is the distance (dissimilarity) between points (data objects), i and j.
- metric: distance that satisfies these properties

Common Properties of a Similarity

- Similarities, also have some well known properties.
 - 1. s(p, q) = 1 (or maximum similarity) only if p = q.
 - 2. s(p, q) = s(q, p) for all p and q. (Symmetry)

where s(p, q) is the similarity between points (data objects), p and q.

Distance of K-means

K-means Objective Function

Sum of Squared Errors(SSE)

$$SSE = \sum_{i=1}^{K} \sum_{x \in C_i} dist^2(c_i, x) \begin{cases} c_i : \text{ ith cluster} \\ \text{the ith cluster} \end{cases}$$

The centroid that minimize the SSE of the cluster is the mean

$$\mathbf{c}_i = \frac{1}{m_i} \sum_{\mathbf{x} \in C_i} \mathbf{x}$$

What if the distance is cosine or L1 distance, rather than Euclidean distance?



Gradient Descent for Euclidean Distance

$$\frac{\partial}{\partial c_k} SSE = \frac{\partial}{\partial c_k} \sum_{i=1}^K \sum_{x \in C_i} (c_i - x)^2$$

the ith chaler
$$=\sum_{i=1}^K\sum_{x\in C_i}\frac{\partial}{\partial c_k}(c_i-x)^2$$

$$=\sum_{k=1}^K\sum_{x\in C_k}\frac{\partial}{\partial c_k}(c_k-x_k)^2$$

$$=\sum_{k=1}^K\sum_{x\in C_k}\frac{\partial}{\partial c_k}(c_k-x_k)^2$$

$$=\sum_{k=1}^K\sum_{x\in C_k}\frac{\partial}{\partial c_k}(c_k-x_k)^2$$

$$= \sum_{k=1}^{\infty} \frac{\left(c_{k} - x_{k} \right)}{\left(c_{k} - x_{k} \right)} = \sum_{k=1}^{\infty} \frac{1}{x \in C_{k}} 2 \times (c_{k} - x_{k}) = 0$$

$$\sum_{x \in C_k} 2 \times (c_k - x_k) = 0 \Rightarrow m_k c_k = \sum_{x \in C_k} x_k \Rightarrow c_k = \frac{1}{m_k} \sum_{x \in C_k} x_k$$

 m_k : number of objects in the k-th cluster

sum of absolute emors

Gradient Descent for

L1 Distance

$$\frac{\partial}{\partial c_k} \text{SAE} = \frac{\partial}{\partial c_k} \sum_{i=1}^K \sum_{x \in C_i} |c_i - x|$$

$$= \sum_{i=1}^K \sum_{x \in C_i} \frac{\partial}{\partial c_k} |c_i - x|$$

$$= \sum_{x \in C_k} \frac{\partial}{\partial c_k} |c_k - x| = 0$$

$$\sum_{x \in C_k} \frac{\partial}{\partial c_k} |c_k - x| = 0 \Rightarrow \sum_{x \in C_k} sign(x - c_k) = 0$$

 c_k : median of objects in the k-th cluster

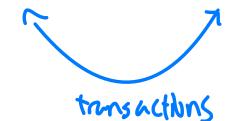
Distance between Transactions

ROCK

- ROCK(RObust Clustering using linKs, '99)
 - Clustering category data
- Major ideas
 - Use links to measure similarity/proximity
 - Not distance-based
 - Computational complexity:
- Algorithm: sampling-based clustering
 - Draw random sample
 - Cluster with links
 - Label data in disk

Similarity Measure in ROCK

- How to cluster set objects
 - Example: how to cluster the following 14 transactions into two clusters
 - Approach:
 - Step 1: Generate proximity matrix
 - Step 2: Hierarchical clustering
 - How to measure the similarity (distance) between two item-sets?
 - Jaccard coefficient
 - $T_1 = \{a, b, c\}, T_2 = \{c, d, e\}$



Similarity Measure in ROCK

- Jaccard coefficient measures for categorical data may not work well
- Example: Two groups (clusters) of transactions
 - C₁ (concept 1) <a, b, c, d, e>: {a, b, c}, {a, b, d}, {a, b, e}, {a, c, d}, {a, c, e}, {a, d, e}, {b, c, d}, {b, c, e}, {b, d, e}, {c, d, e}
 - C_2 . (concept 2) <a, b, f, g>: {a, b, f}, {a, b, g}, {a, f, g}, {b, f, g}
- Jaccard co-efficient may lead to wrong clustering result
 - C₁: 0.2 ({a, b, c}, {b, d, e}) to 0.5 ({a, b, c}, {a, b, d})
 - C₁ & C₂: could be as high as 0.5 ({a, b, c}, {a, b, f})

Link Measure in ROCK

- Links: # of common neighbors (link threshold Jaccard >= 0.5)
 - C₁ <a, b, c, d, e>: {a, b, c}, {a, b, d}, {a, b, e}, {a, c, d}, {a, c, e}, {a, d, e}, {b, c, d}, {b, c, e}, {b, d, e}, {c, d, e}
 - C_2 <a, b, f, g>: {a, b, f}, {a, b, g}, {a, f, g}, {b, f, g}
 - $link({a,b,c}_1,{c,d,e}_1) = 4$, 4 common neighbors
 - {a, c, d}, {a, c, e}, {b, c, d}, {b, c, e}
 - $link({a,b,c}_1,{a,b,f}_2) = 3$, 3 common neighbors
 - {a, b, d}, {a, b, e}, {a, b, g}
 - $link({a,f,g}₂, {a,b,g}₂) = 2, 2 common neighbors$
 - {a,b,f}, {b,f,g}
 - $link({a,f,g}_2,{a,b,c}_1) = 0$, 0 common neighbors
- Link is a better measure than Jaccard coefficient

Distance between Sequences?

d(abbc, babb) = ?

Distance between Time Series?

```
d(<300, 250, 280, 350>, <290, 280, 350, 300>) = ?
```

Cluster Evaluation

Cluster Evaluation

- Cluster evaluation is not well-developed.
- Sometimes, cluster analysis is conducted as a part of an exploratory data analysis. Hence cluster evaluation seems to be unnecessary.
- There are different types of clusters. Each type requires different evaluation measure.
- Nonetheless, cluster evaluation should be part of any cluster analysis.
 - To avoid finding patterns in noise
 - To determine the clustering tendency of dataset
 - To determine the number of clusters
 - To compare clustering algorithms
 - To compare clustering results (internally, externally)

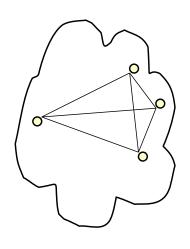
Cluster Evaluation (cont.)

- Evaluation measures
 - Unsupervised (internal indices): to measure the goodness of a clustering structure without respect to external information.
 - Cluster cohesion
 - Cluster separation
 - Supervised (external indices): to measure the extent to which cluster labels match externally supplied class labels.

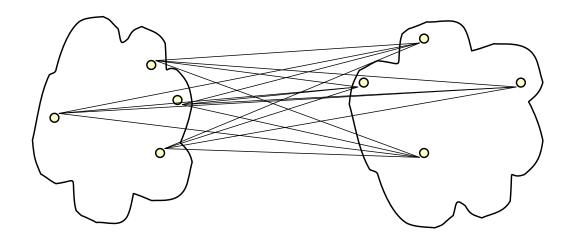
Unsupervised Cluster Evaluation

- Graph-based view: focusing on painwise relationships $overall \ validity = \sum_{i=1}^K w_i \times validity(C_i) \ (W_i: weights)$

 - $cohesion(C_i) = \sum_{x,y \in C_i} proximity(x,y)$
 - $separation(C_i, C_j) = \sum_{x \in C_i, y \in C_j} proximity(x, y)$



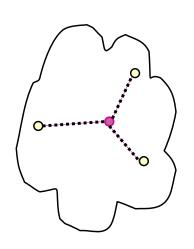


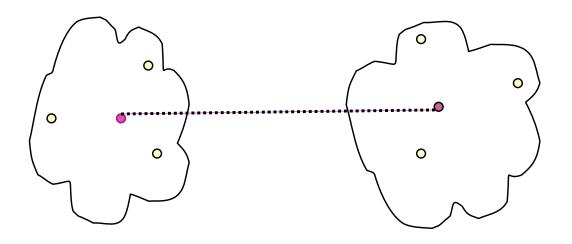


separation

Unsupervised Cluster Evaluation (cont.)

- · Prototype-based view : focusing on representative points
 - overall validity = $\sum_{i=1}^{K} w_i \times validity(C_i)$
 - $cohesion(C_i) = \sum_{x \in C_i} proximity(x, C_i)$
 - $separation(C_i, C_j) = proximity(C_i, C_j)$
 - $separation(C_i) = proximity(C_i, c)$, c is overall centroid





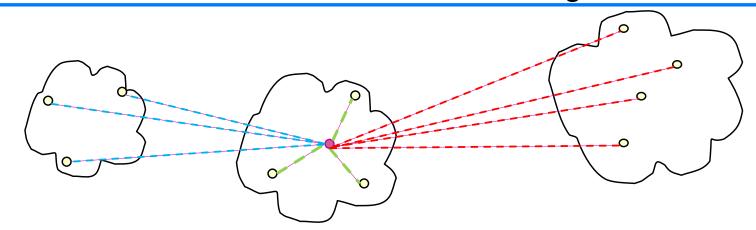
cohesion

separation

Evaluating Individual Object

- Evaluation individual object within a cluster
 - Silhouette coefficient : a measure of
 how similar an object is to its own cluster (cohesion)
 compared to other clusters (separation)
 - Silhouette coefficient for an object i, $s_i = \frac{b_i a_i}{\max(a_i, b_i)}$, [-1, 1]
 - a_i: average distance to all objects within cluster
 - b_i: minimum distance to other clusters

where distance to other cluster is the average distance



Silhouette Coefficient:

Silhouette Coefficient or silhouette score is a metric used to calculate the goodness of a clustering technique. Its value ranges from -1 to 1.

1: Means clusters are well apart from each other and clearly distinguished.

0: Means clusters are indifferent, or we can say that the distance between clusters is not significant.

1. Means clusters are assigned in the wrong way.

1. Means clusters are assigned in the wrong way.

3.
$$b_i \rightarrow a_i$$

3. $b_i = a_i$

4. $b_i \rightarrow a_i$

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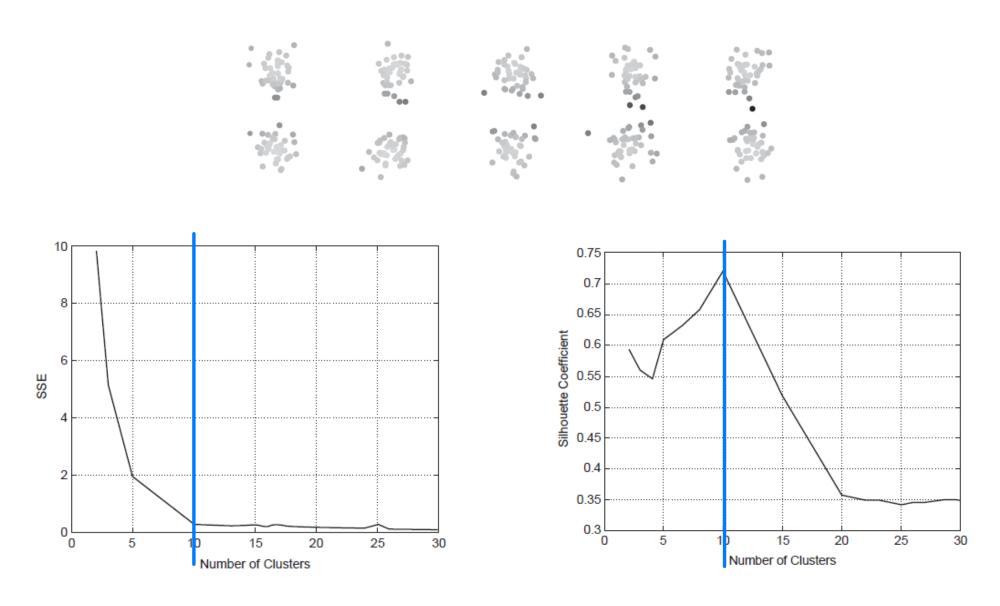
6. $b_i \rightarrow a_i$

8. $b_i \rightarrow a_i$

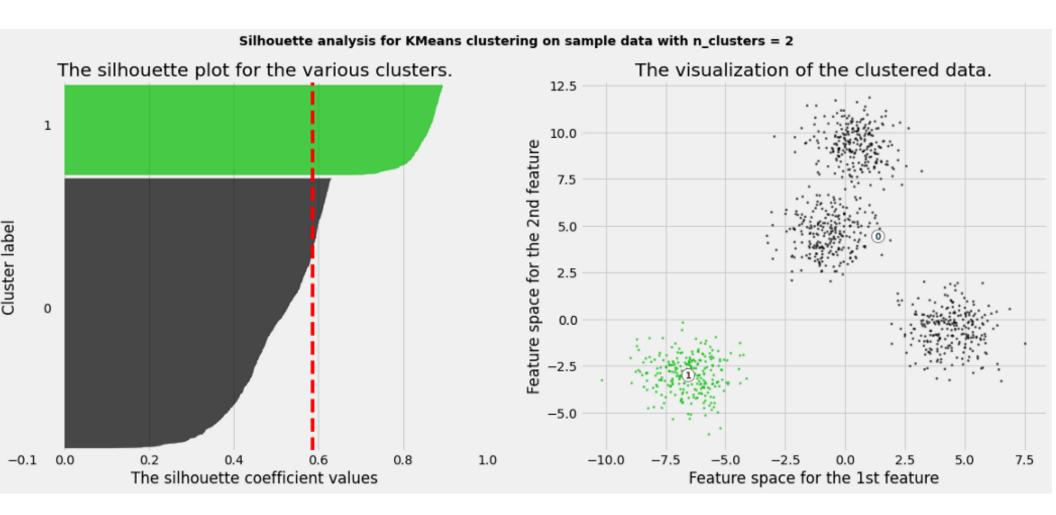
9. $b_i \rightarrow a_i$

1. $b_i \rightarrow$

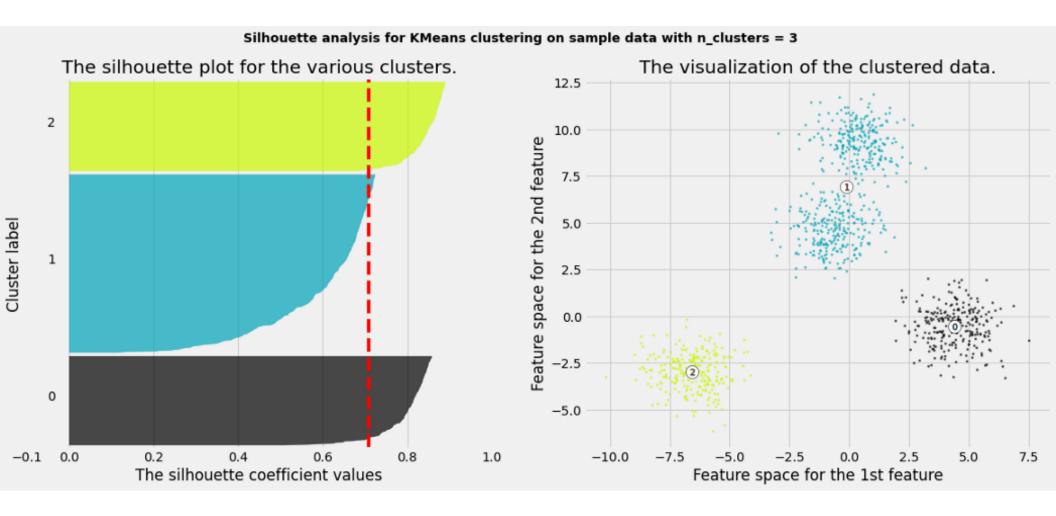
Determining the Number of Clusters

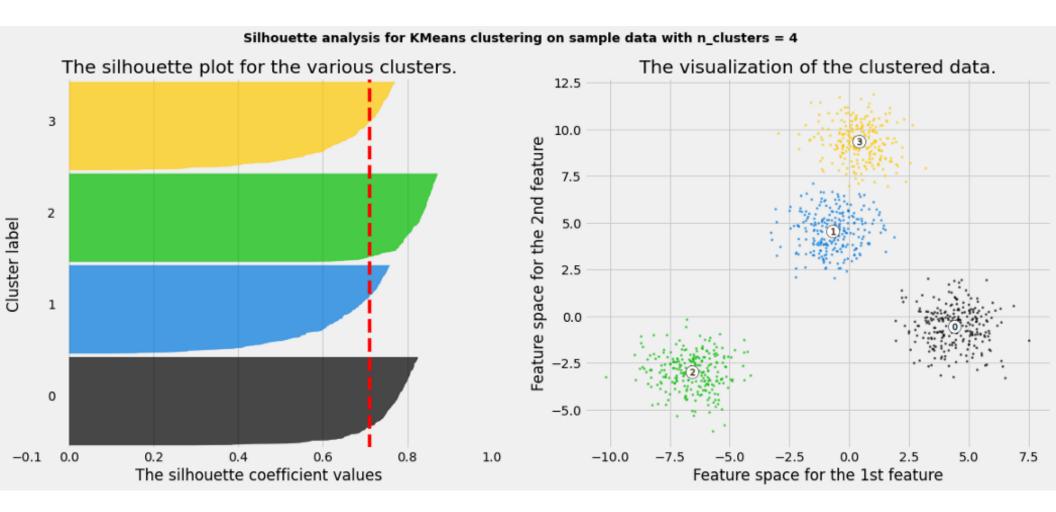


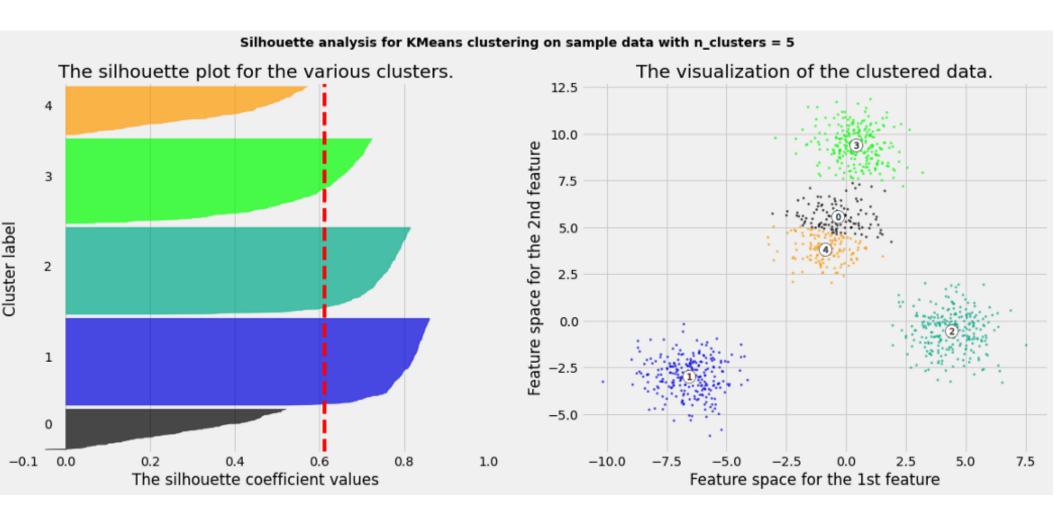
Elbow method



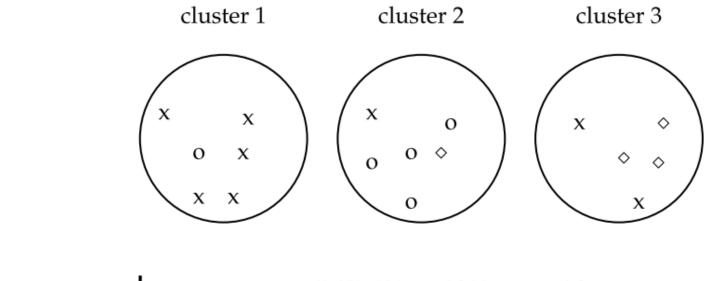
ref: https://medium.com/mlearning-ai/stop-using-the-elbow-method-to-compute-optimal-clusters-in-k-means-clustering-1f572c587d2e







Supervised Cluster Evaluation



	purity	NMI	RI	F_5
lower bound	0.0	0.0	0.0	0.0
maximum	1	1	1	1
value	0.71	0.36	0.68	0.46

(ref: Introduction to Information Retrieval by Manning et al.)

Supervised Cluster Evaluation: Purity

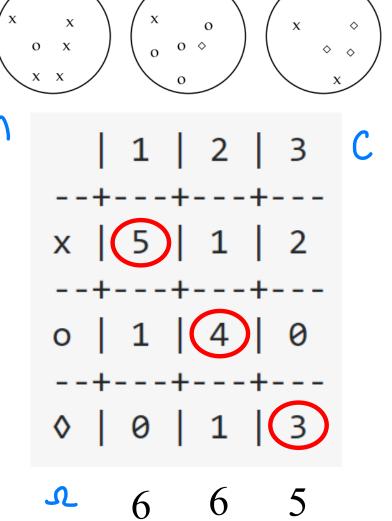
purity
$$(\Omega, \mathbb{C}) = \frac{1}{N} \sum_{k} \max_{j} |\omega_{k} \cap c_{j}|$$

$$\Omega = \{\omega_{1}, \omega_{2}, \dots, \omega_{K}\}$$

$$\mathbb{C} = \{c_{1}, c_{2}, \dots, c_{J}\}$$

cluster 1

purity(
$$\Omega$$
, \mathbb{C}) = $\frac{1}{N} \sum_{k} \max_{j} |\omega_{k} \cap c_{j}|$
= $\frac{1}{(6+6+5)} * (5+4+3)$
= 0.71

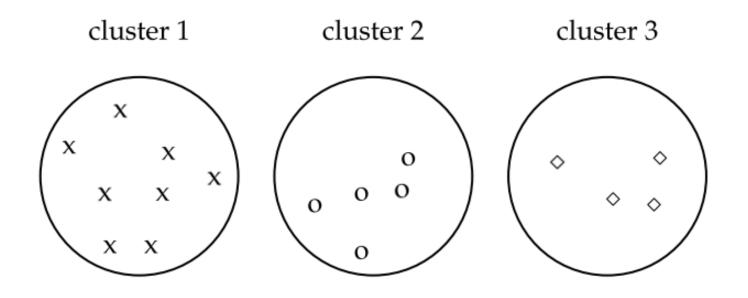


cluster 2

cluster 3

Supervised Cluster Evaluation: Purity (cont.)

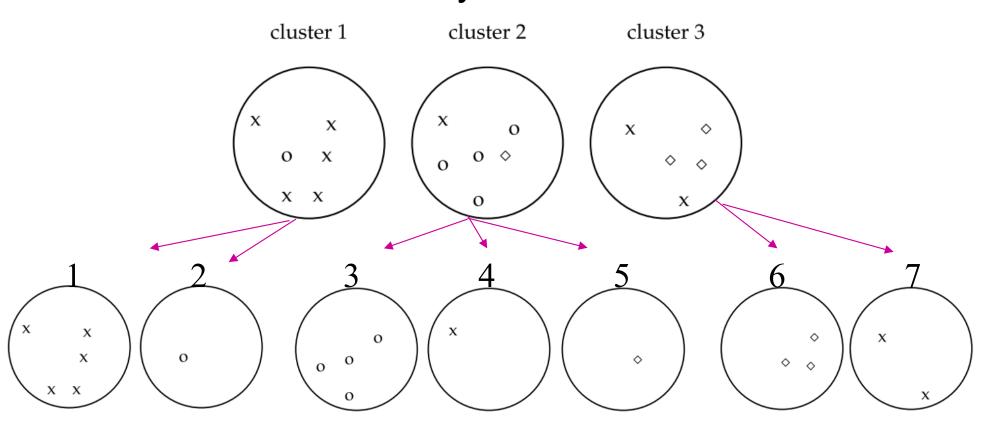
Condition for Purity = 1



purity(
$$\Omega$$
, \mathbb{C}) = $\frac{1}{N} \sum_{k} \max_{j} |\omega_k \cap c_j|$
= $\frac{1}{(8+5+4)} * (8+5+4)$
= 1

Supervised Cluster Evaluation: Purity (cont.)

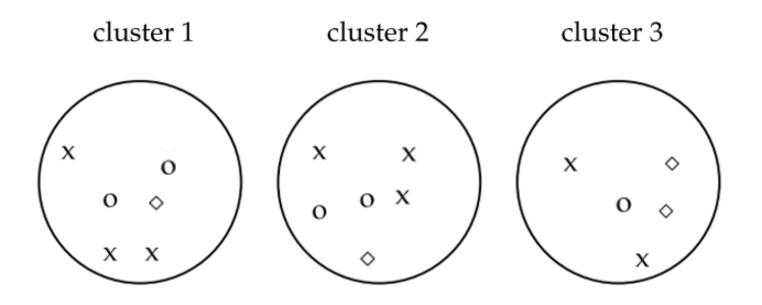
Other condition for Purity = 1



purity(
$$\Omega$$
, \mathbb{C}) = $\frac{1}{N} \sum_{k} \max_{j} |\omega_{k} \cap c_{j}|$
= $\frac{1}{17} * (5 + 1 + 4 + 1 + 1 + 3 + 2) = 1$

Supervised Cluster Evaluation: Purity (cont.)

Purity for worse clustering



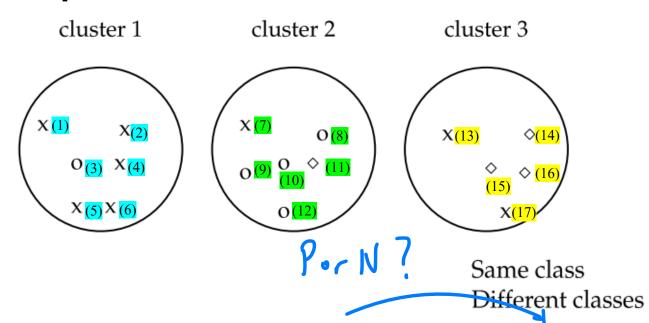
purity(
$$\Omega$$
, \mathbb{C}) = $\frac{1}{N} \sum_{k} \max_{j} |\omega_k \cap c_j|$
= $\frac{1}{17} * (3 + 3 + 2) = 0.47$

• **Purity**: Purity is a measure of the extent to which clusters contain a single class. [38] Its calculation can be thought of as follows: For each cluster, count the number of data points from the most common class in said cluster. Now take the sum over all clusters and divide by the total number of data points. Formally, given some set of clusters M and some set of classes D, both partitioning N data points, purity can be defined as:

$$rac{1}{N}\sum_{m\in M}\max_{d\in D}|m\cap d|$$

This measure doesn't penalize having many clusters, and more clusters will make it easier to produce a high purity. A purity score of 1 is always possible by putting each data point in its own cluster. Also, purity doesn't work well for imbalanced data, where even poorly performing clustering algorithms will give a high purity value. For example, if a size 1000 dataset consists of two classes, one containing 999 points and the other containing 1 point, then every possible partition will have a purity of at least 99.9%.

Supervised Cluster Evaluation: Rand Index



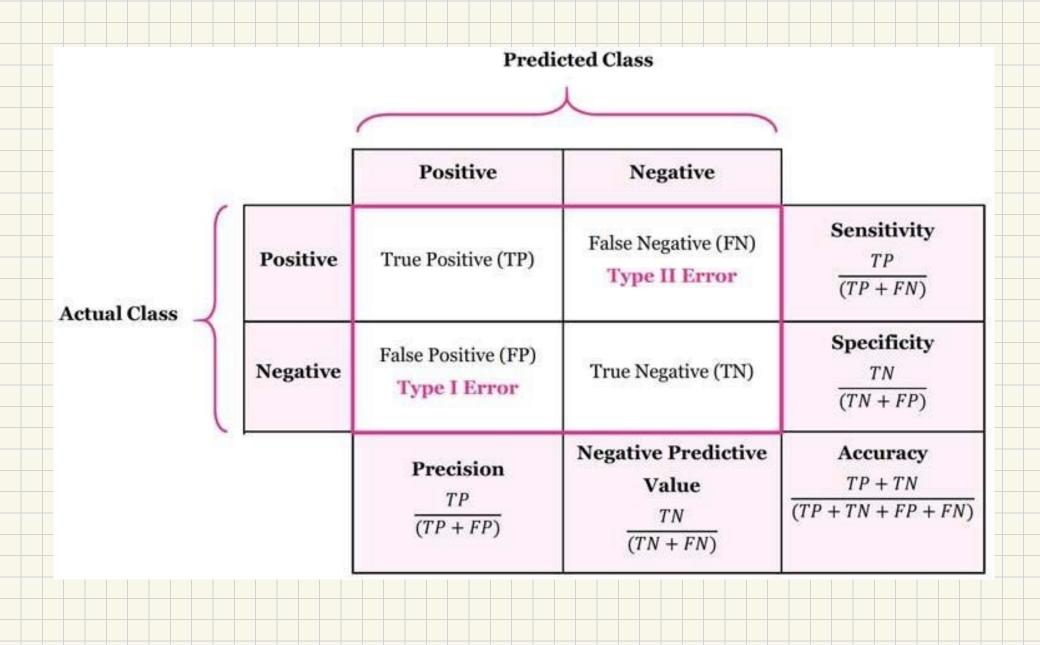
Same cluster	Different clusters
TP = 20	FN = 24
FP = 20	TN = 72

C(17,2)	Pair	(x,y)	Same Cluster	Same Class	
1	1	2	Т	Т	TP
2	1	3	Т	F	FP
3	1	7	F	Т	FN
4	1	8	F	F	TN
5	1	11	F	F	TN
•••					
136			Т	F	FP

$$RI = \frac{TP + TN}{TP + FP + FN + TN}$$

$$RI = \frac{20+72}{(20+20+24+72)}$$

$$= 0.68$$



Conclusions

- Quality factors
 - Similarity measure and its implementation
 - Euclidean distance
 - City block distance
 - Cosine
 - •
 - definition and representation of cluster chosen
 - Means
 - Medoids
 - Nearest, Farest
 - clustering algorithm

Conclusions (cont.)

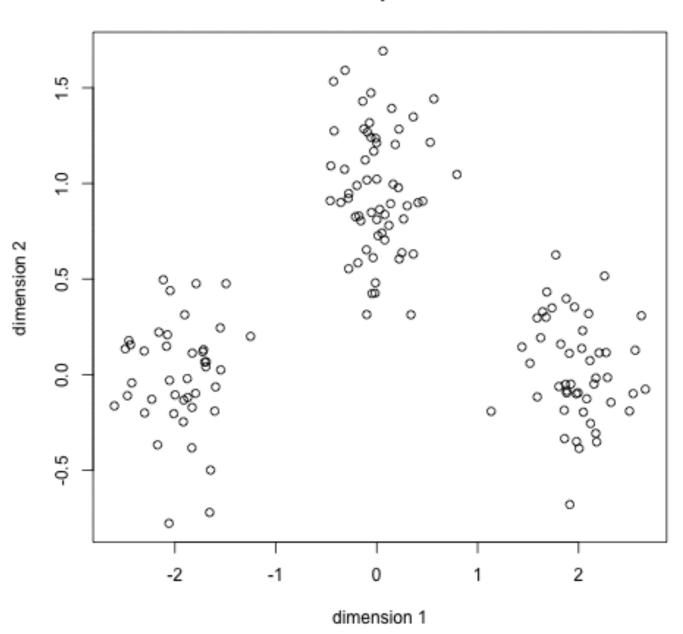
- Quality factors
 - Similarity measure and its implementation
 - definition and representation of cluster chosen
 - clustering algorithm
 - K-means, K-medoids
 - Single-Link, Complete-Link, Average-Link, Chameleon
 - DBSCAN
 - EM

Conclusions (cont.)

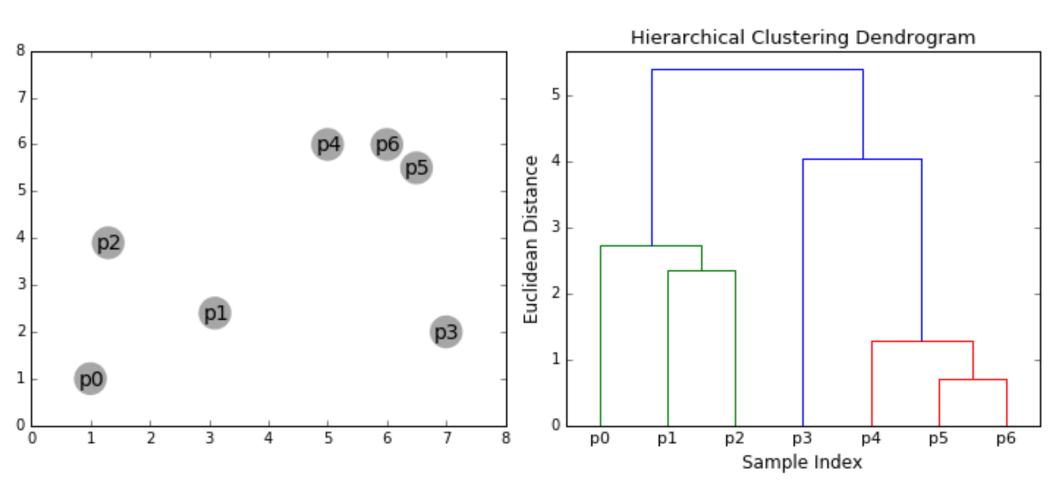
- Which clustering algorithm?
 - Type of clustering produced.
 - Biological Taxonomy: Hierarchical clustering
 - Characteristics of clusters: shape, sizes, densities
 - Characteristics of data set and attributes
 - K-means: data matrix
 - Noise & outlier
 - Number of objects (scalability)
 - Number of attributes
 - Cluster interpretation
 - Algorithmic considerations: ordered, parameters

K-means

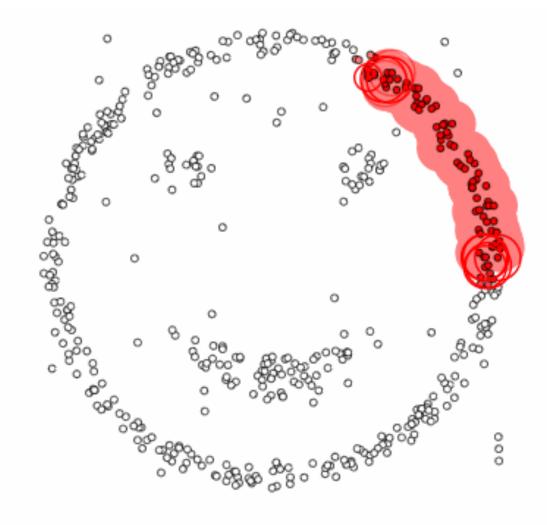
step 0



Hierarchical Clustering



DBSCAN



epsilon = 1.00 minPoints = 4

Restart

Pause

GMM

