

CSE 473: Pattern Recognition

Syntactic Pattern Recognition

Extension to Graph Matching Approach

- ▶ An attributed graph $G = \{N, P, R\}$ is a 3-tuple where
 - N is a set of nodes,
 - P is a set of properties of these nodes.
 - R is a set of relations between nodes.

Assignment of nodes:

Let $p_q^i(n)$ denote the value of the q'th property of node n of graph G_i .

Assignment of nodes:

Let $p_q^i(n)$ denote the value of the q'th property of node n of graph G_i .

• Nodes $n_1 \in N_1$ and $n_2 \in N_2$ are said to form an assignment (n_1, n_2) if

$$p_q^1(n_1) \sim p_q^2(n_2)$$

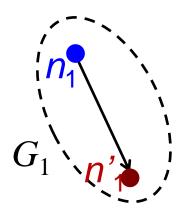
where " \sim " denotes similarity.

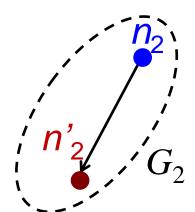
- Let $\underline{r_j^i(n_x,n_y)}$ denote the j'th relation involving nodes $n_x, n_y \in N_i$.
- ► Two assignments (n₁, n₂) and (n'₁, n'₂) are considered compatible if

$$r_j^1(n_1, n_1') \sim r_j^2(n_2, n_2') \quad \forall j.$$

- Let $\underline{r_j^i(n_x,n_y)}$ denote the j'th relation involving nodes $n_x,n_y\in N_i$.
- ► Two assignments (n₁, n₂) and (n'₁, n'₂) are considered compatible if

$$r_j^1(n_1, n_1') \sim r_j^2(n_2, n_2') \quad \forall j.$$





- Let $\underline{r_j^i(n_x,n_y)}$ denote the j'th relation involving nodes $n_x,n_y\in N_i$.
- ► Two assignments (n₁, n₂) and (n'₁, n'₂) are considered compatible if

$$r_j^1(n_1,n_1') \sim r_j^2(n_2,n_2') \quad \forall j.$$

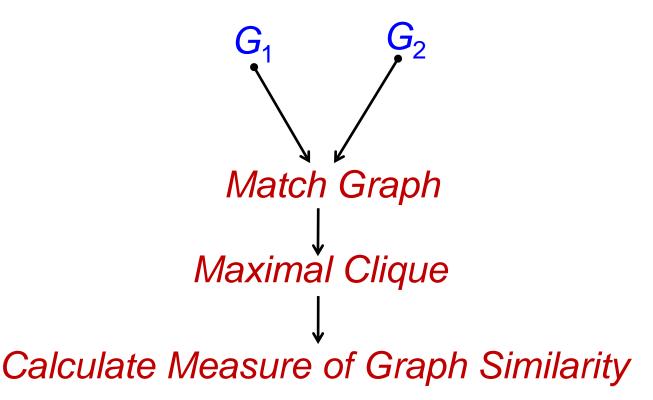
- Let $\underline{r_j^i(n_x,n_y)}$ denote the j'th relation involving nodes $n_x,n_y\in N_i$.
- ► Two assignments (n₁, n₂) and (n'₁, n'₂) are considered compatible if

$$r_j^1(n_1,n_1') \sim r_j^2(n_2,n_2') \quad \forall j.$$

Assignment and Isomorphism:

• Two attributed graphs G_1 and G_2 are isomorphic if there exists a set of 1:1 assignments of nodes in G_1 to nodes in G_2 such that all assignments are compatible.

A strategy for measuring the similarity between two attributed graphs is to find node pairings using the cliques of a match graph.



- ▶ A *match graph* is formed from two graphs G_1 and G_2 as follows:
 - Nodes of the match graph are assignments from G_1 to G_2
 - An edge in the match graph exists between two nodes if the corresponding assignments are compatible.

- ▶ A *match graph* is formed from two graphs G_1 and G_2 as follows:
 - ▶ Nodes of the match graph are assignments from G_1 to G_2 .
 - An edge in the match graph exists between two nodes if the corresponding assignments are compatible.
- A clique of a graph is a totally connected subgraph.
- A maximal clique is not included in any other clique.

Approaches in Matching Through Attributed Graph

- Steps
 - draw attributed graphs from the patterns
 - draw match graphs from the attributed graph
 - find the maximum clique from the match graph
 - calculate the similarity

Input:

- X: an initial clique (possibly empty)
- Y: the graph

Output:

The set of all maximal cliques

```
Procedure clique (X, Y)

Form Y – X;

If a node y in Y – X is connected to all nodes of X,

Then return cliques (X U {y}, Y) U cliques (X, Y-{y})

Else return X

End
```

```
Procedure clique (X, Y)

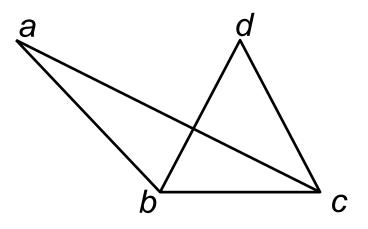
Form Y – X;

If a node y in Y – X is connected to all nodes of X,

Then return cliques (X U {y}, Y) U cliques (X, Y-{y})

Else return X

End
```



```
Procedure clique (X, Y)

Form Y - X;

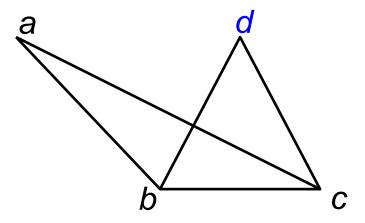
If a node y in Y - X is connected to all nodes of X,

Then return cliques (X U {y}, Y) U cliques (X, Y-{y})

Else return X

End

Find clique (d, Y)?
```



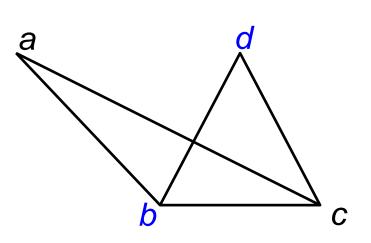
```
Procedure clique (X, Y)

Form Y – X;

If a node y in Y – X is connected to all nodes of X,

Then return cliques (X U {y}, Y) U cliques (X, Y-{y})

Else return X
```



clique
$$(d, Y) = clique (\{d, b\}, Y) \cup clique (d, \{a, c, d\})$$

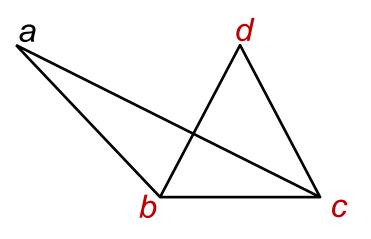
```
Procedure clique (X, Y)

Form Y – X;

If a node y in Y – X is connected to all nodes of X,

Then return cliques (X U {y}, Y) U cliques (X, Y-{y})

Else return X
```



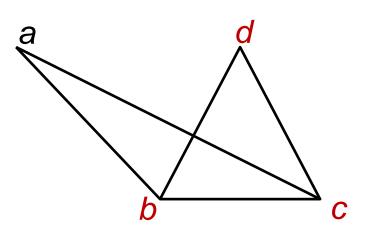
```
Procedure clique (X, Y)

Form Y - X;

If a node y in Y - X is connected to all nodes of X,

Then return cliques (X \cup \{y\}, Y) \cup cliques (X, Y - \{y\})

Else return X
```



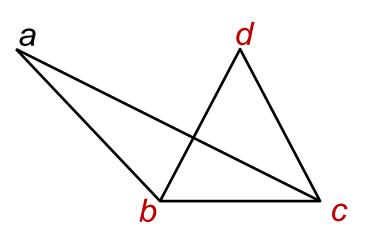
```
Procedure clique (X, Y)

Form Y – X;

If a node y in Y – X is connected to all nodes of X,

Then return cliques (X U {y}, Y) U cliques (X, Y-{y})

Else return X
```



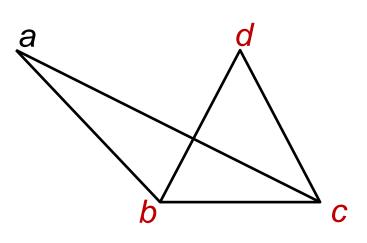
```
Procedure clique (X, Y)

Form Y – X;

If a node y in Y – X is connected to all nodes of X,

Then return cliques (X U {y}, Y) U cliques (X, Y-{y})

Else return X
```



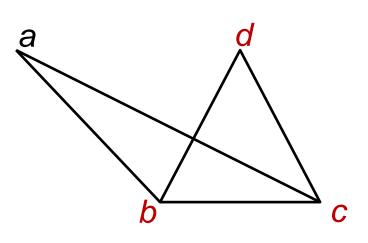
```
Procedure clique (X, Y)

Form Y – X;

If a node y in Y – X is connected to all nodes of X,

Then return cliques (X U {y}, Y) U cliques (X, Y-{y})

Else return X
```



clique (d, Y) = clique (
$$\{d, b\}$$
, Y) U

clique (d, $\{a, c, d\}$)

clique ($\{d, b\}$, Y) = $\{d, b, c\}$ U $\{d, b\}$

= $\{d, b, c\}$

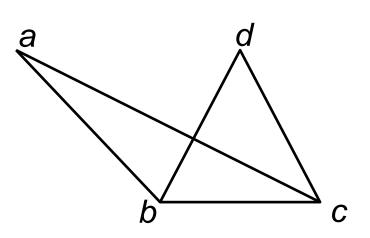
```
Procedure clique (X, Y)

Form Y – X;

If a node y in Y – X is connected to all nodes of X,

Then return cliques (X U {y}, Y) U cliques (X, Y-{y})

Else return X
```



clique
$$(d, Y) = \{d, b, c\} \cup \{d, b\} \cup clique (d, \{a, c, d\})$$

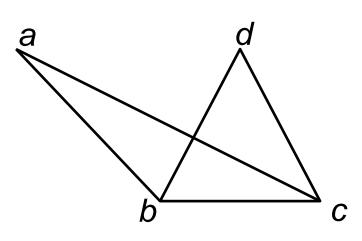
```
Procedure clique (X, Y)

Form Y - X;

If a node y in Y - X is connected to all nodes of X,

Then return cliques (X \cup \{y\}, Y) \cup cliques (X, Y - \{y\})

Else return X
```



```
clique (d, Y) = {d, b, c} U {d, b} U
clique (d, {a, c, d})
clique (d, {a, c, d})
= clique ({d, c}, {a, c, d})
U clique (d, {a, d})
```

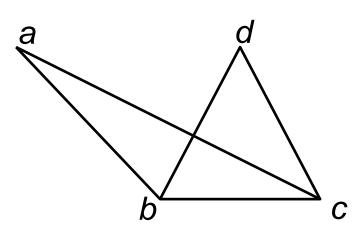
```
Procedure clique (X, Y)

Form Y – X;

If a node y in Y – X is connected to all nodes of X,

Then return cliques (X U {y}, Y) U cliques (X, Y-{y})

Else return X
```



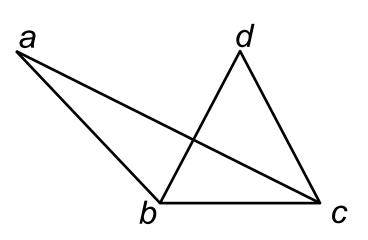
```
Procedure clique (X, Y)

Form Y – X;

If a node y in Y – X is connected to all nodes of X,

Then return cliques (X U {y}, Y) U cliques (X, Y-{y})

Else return X
```



clique
$$(d, Y) = \{d, b, c\} \cup \{d, b\}$$

 $\cup \{d, c\} \cup \{d\}$

```
Procedure clique (X, Y)

Form Y - X;

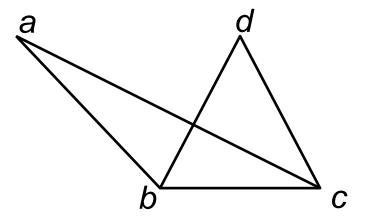
If a node y in Y - X is connected to all nodes of X,

Then return cliques (X \cup \{y\}, Y) \cup cliques (X, Y-\{y\})

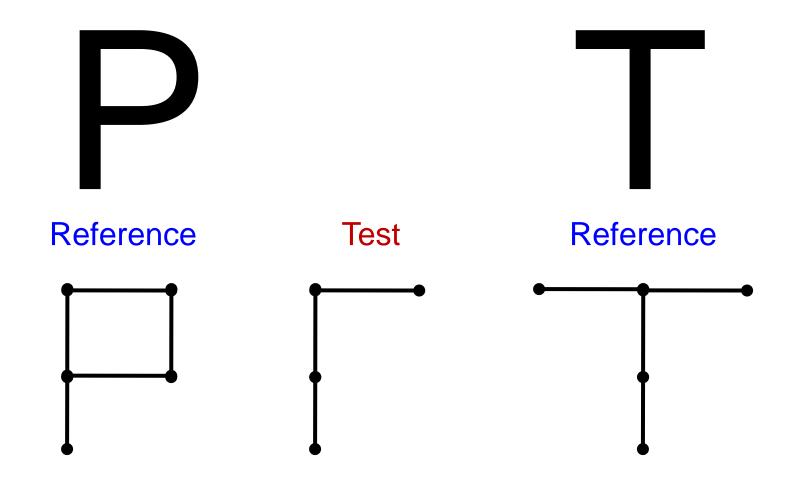
Else return X

End

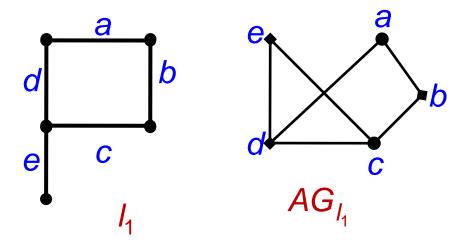
The maximal clique is = \{d, b, c\}
```



Reference Reference



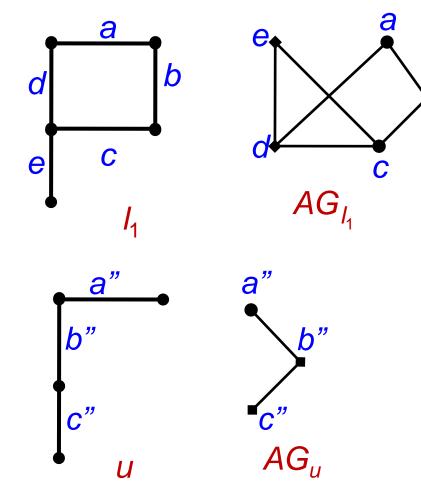
Find Attributed Graph for all patterns

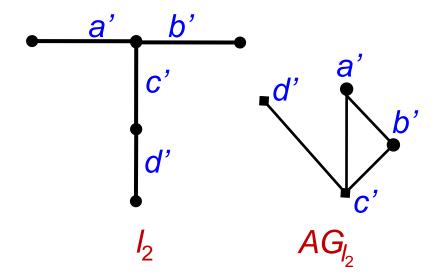


- Horizontal line
- ♦ Vertical line

Relation: —— connected

Find Attributed Graph for all patterns

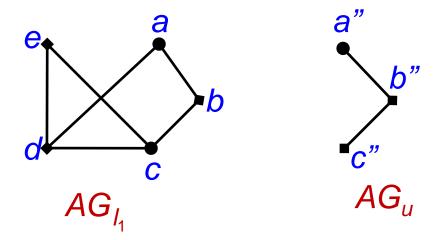




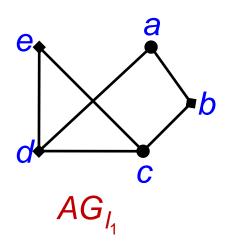
- Horizontal line
- ♦ Vertical line

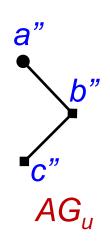
Relation: —— connected

Find Matched Graph between AGI₁ and AG_u



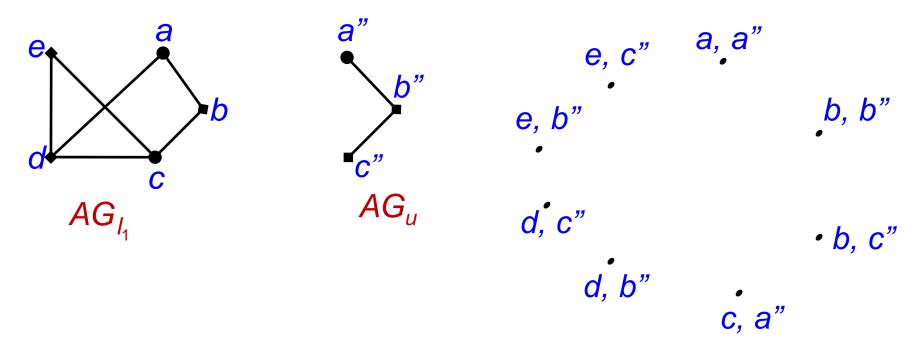
Find Matched Graph between AGI_1 and AG_u





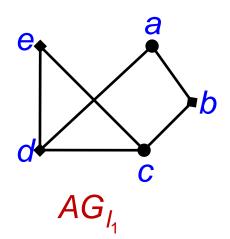
Find all assignments between AGI_1 and AG_{ij} :

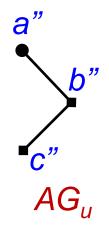
Find Matched Graph between AGI₁ and AG_u

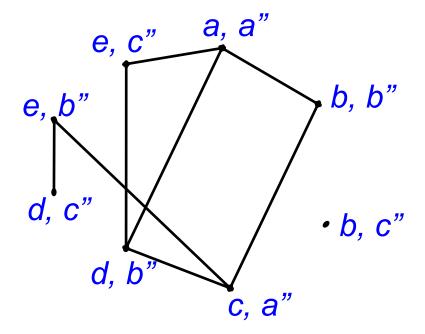


Find all assignments between AGI_1 and AG_{II}

Find Matched Graph between AGI_1 and AG_u

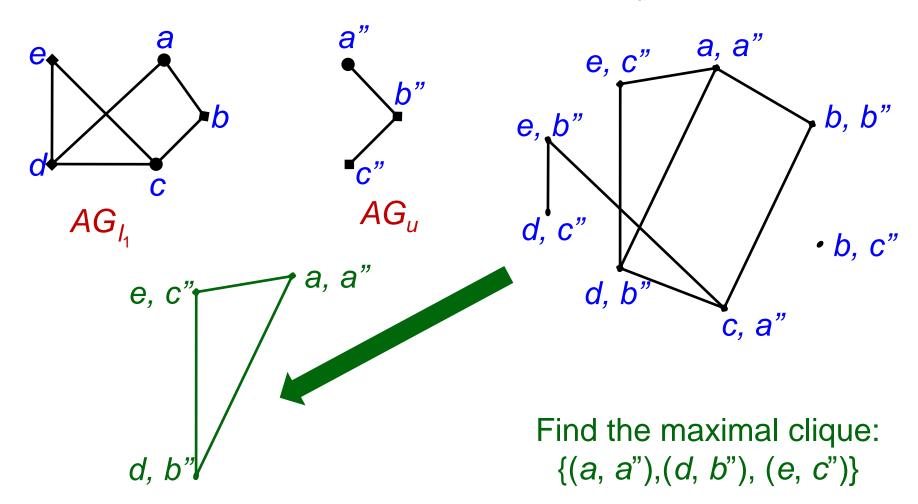




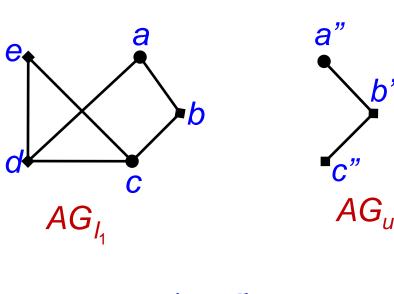


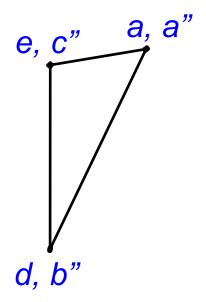
Connect the compatible assignments

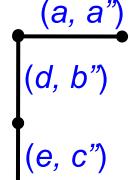
Find Matched Graph between AGI₁ and AG_u



Find Matched Graph between AGI₁ and AG₁₁



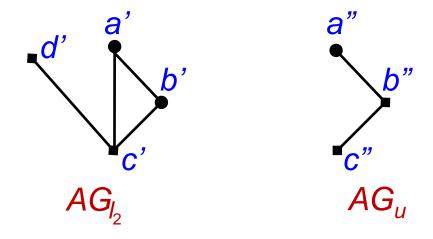




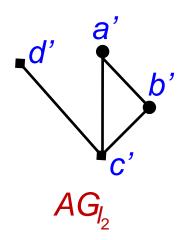


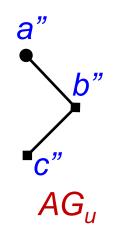
Visual Representation

Find Matched Graph between AGI₁ and AG_u



Find Matched Graph between AGI_1 and AG_u



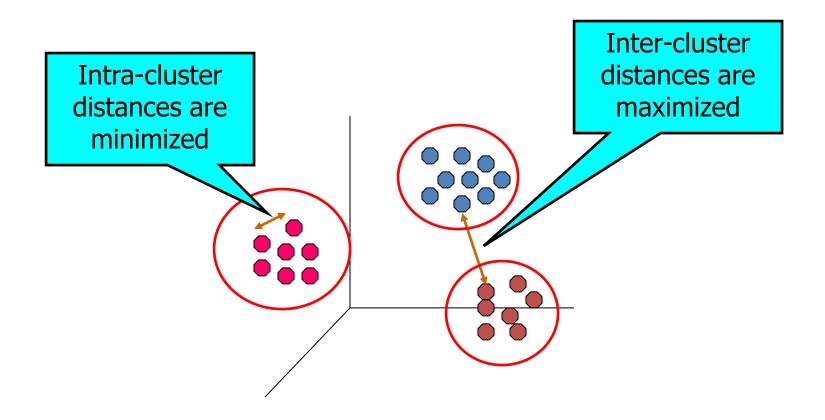


Find all assignments between AGI_2 and AG_{ii} :

Unsupervised Learning:Clustering

What is Cluster Analysis?

 Finding groups of objects such that the objects in a group will be similar (or related) to one another and different from (or unrelated to) the objects in other groups



Applications

Understanding

- Biological taxonomy
- Group related documents for browsing
- Group genes and proteins that have similar functionality
- Group stocks with similar price fluctuations

Summarization

Reduce the size of large data sets

Data Compression

Vector quantization

Finding nearest neighbor

Applications ...

- Hypothesis generation
 - To infer some hypothesis
- Hypothesis testing
 - To verify an existing hypothesis
 - Example: 'big companies invest overseas'
- Prediction based on groups
 - Predict unknown patterns

What is not Cluster Analysis?

- Supervised classification
 - Have class label information
- Simple segmentation
 - Dividing students into different registration groups alphabetically, by last name
- Results of a query
 - Groupings are a result of an external specification

Clustering Basis

Basic Concepts

a clustering criterion must first be adopted.

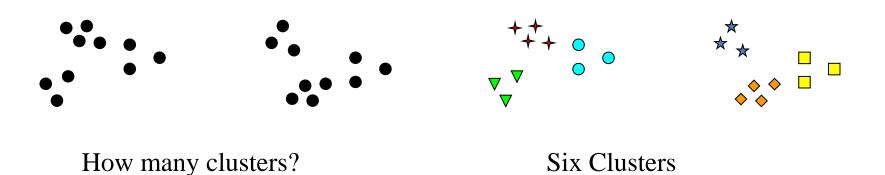
Different criteria lead to different clusters.

Notion of a Cluster can be Ambiguous

 Depending on the similarity measure, the clustering criterion and the clustering algorithm, different clusters may result. Subjectivity is a reality to live with from now on.

Notion of a Cluster can be Ambiguous

 Depending on the similarity measure, the clustering criterion and the clustering algorithm, different clusters may result. Subjectivity is a reality to live with from now on.





Two Clusters Four Clusters

Notion of a Cluster can be Ambiguous

- Let these animals to be clustered
 - Blue shark, sheep, cat, Dog, Lizard, sparrow, viper, seagull, gold fish, frog, red mullet

A real example

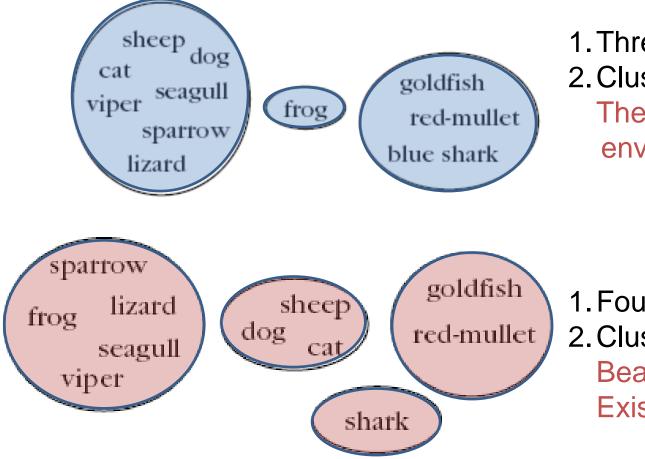
Blue shark, sheep, cat, dog Lizard, sparrow, viper, seagull, gold fish, frog, red mullet

- 1. Two clusters
- 2. Clustering criterion:
 How mammals bear
 their progeny

Gold fish, red mullet, blue shark Sheep, sparrow, dog, cat, seagull, lizard, frog, viper

- 1. Two clusters
- 2. Clustering criterion: Existence of lungs

A real example



- 1. Three clusters
- 2. Clustering criterion:

Their living environment

- 1. Four clusters
- 2. Clustering criterion:

Bear progeny and Existence of lungs

Clustering Task Stages

- Feature Selection: Information rich features-Parsimony
- Proximity Measure: This quantifies the term similar or dissimilar.
- Clustering Criterion: This consists of a cost function or some type of rules.
- Clustering Algorithm: This consists of the set of steps followed to reveal the structure, based on the similarity measure and the adopted criterion.
- Validation of the results.
- Interpretation of the results.

Types of Features

- With respect to their <u>domain</u>
 - Continuous (the domain is a continuous subset of \Re).
 - Discrete (the domain is a finite discrete set).
 - Binary or dichotomous (the domain consists of two possible values).
- With respect to the relative significance of the values they take
 - Nominal (the values code states, e.g., the home district of an individual).
 - Ordinal (the values are meaningfully ordered, e.g., the rating of the services of a hotel (poor, good, very good, excellent)).
 - Interval-scaled (the difference of two values is meaningful but their ratio is meaningless, e.g., temperature).
 - Ratio-scaled (the ratio of two values is meaningful, e.g., weight).

Hard Clustering: Each point belongs to a single cluster

• Let
$$X = \{\underline{x}_1, \underline{x}_2, ..., \underline{x}_N\}$$

• An m-clustering R of X, is defined as the partition of X into m sets (clusters), $C_1, C_2, ..., C_m$, so that

$$-C_i \neq \emptyset, i = 1, 2, ..., m$$

$$- \bigcup_{i=1}^{m} C_i = X$$

$$-C_i \cap C_j = \emptyset, i \neq j, i, j = 1, 2, ..., m$$

– In addition, data in C_i are more similar to each other and less similar to the data in the rest of the clusters.

 Fuzzy clustering: Each point belongs to all clusters up to some degree.

A fuzzy clustering of X into m clusters is characterized by m functions

- u_j is the representative of *j*th cluster
- $u_j: \underline{x} \to [0,1], j = 1,2,...,m$

These are known as membership functions. Thus, each \underline{x}_i belongs to any cluster "up to some degree", depending on the value of

$$u_{j}(\underline{x}_{i}), j = 1,2,...,m$$

 $u_j(\underline{x}_i)$ close to $1 \Rightarrow$ high grade of membership of \underline{x}_i to cluster j.

$$u_j(\underline{x}_i)$$
 close to $0 \Rightarrow$

low grade of membership.

 Fuzzy clustering: Each point belongs to all clusters up to some degree.

A fuzzy clustering of X into m clusters is characterized by m functions

- u_j is the representative of *j*th cluster
- $u_j: \underline{x} \to [0,1], j = 1,2,...,m$
- $\sum_{j=1}^{m} u_j(\underline{x}_i) = 1, i = 1, 2, ..., N$
- $0 < \sum_{i=1}^{N} u_{j}(\underline{x}_{i}) < N, \ j = 1, 2, ..., m$

- Between vectors
 - Dissimilarity measure (between vectors of X) is a function

$$d: X \times X \longrightarrow \mathfrak{R}$$

with the following properties

$$\exists d_0 \in \Re: \ -\infty < d_0 \le d(\underline{x}, \underline{y}) < +\infty, \ \forall \underline{x}, \underline{y} \in X$$

•
$$d(\underline{x},\underline{x}) = d_0, \ \forall \underline{x} \in X$$

•
$$d(\underline{x}, \underline{y}) = d(\underline{y}, \underline{x}), \ \forall \underline{x}, \underline{y} \in X$$

If, in addition

•
$$d(\underline{x}, \underline{y}) = d_0$$
 if and only if $\underline{x} = \underline{y}$

•
$$d(\underline{x},\underline{z}) \le d(\underline{x},\underline{y}) + d(\underline{y},\underline{z}), \ \forall \underline{x},\underline{y},\underline{z} \in X$$

(triangular inequality)

d is called a metric dissimilarity measure.

- Similarity measure (between vectors of X) is a function

$$s: X \times X \longrightarrow \Re$$

with the following properties

$$\exists s_0 \in \Re: -\infty < s(\underline{x}, \underline{y}) \le s_0 < +\infty, \ \forall \underline{x}, \underline{y} \in X$$

•
$$s(\underline{x},\underline{x}) = s_0, \ \forall \underline{x} \in X$$

$$\cdot s(\underline{x}, \underline{y}) = s(\underline{y}, \underline{x}), \ \forall \underline{x}, \underline{y} \in X$$

If, in addition

•
$$s(\underline{x}, \underline{y}) = s_0$$
 if and only if $\underline{x} = \underline{y}$

•
$$s(\underline{x}, \underline{y})s(\underline{y}, \underline{z}) \leq [s(\underline{x}, \underline{y}) + s(\underline{y}, \underline{z})]s(\underline{x}, \underline{z}), \ \forall \underline{x}, \underline{y}, \underline{z} \in X$$

s is called a metric similarity measure.

Between sets

Let
$$D_i \subset X$$
, $i=1,...,k$ and $U=\{D_1,...,D_k\}$

A proximity measure \wp on U is a function

$$\wp: U \times U \longrightarrow \Re$$

Proximity Measures Between Points/Vectors

- Real-valued vectors
 - Dissimilarity measures (DMs)
 - ullet Weighted l_p metric DMs

$$d_p(\underline{x},\underline{y}) = \left(\sum_{i=1}^l w_i \mid x_i - y_i \mid^p\right)^{1/p}$$

Interesting instances are obtained for

- -p=1 (weighted Manhattan norm)
- -p=2 (weighted Euclidean norm)
- $-p = \infty (d_{\infty}(\underline{x}, \underline{y}) = \max_{1 \le i \le l} w_i | x_i y_i |)$

Proximity Measures Between Vectors

- Similarity measures
 - Inner product

$$S_{inner}(\underline{x}, \underline{y}) = \underline{x}^T \underline{y} = \sum_{i=1}^l x_i y_i$$

Tanimoto measure

$$s_T(\underline{x}, \underline{y}) = \frac{\underline{x}^T \underline{y}}{\|\underline{x}\|^2 + \|\underline{y}\|^2 - \underline{x}^T \underline{y}}$$

- Let $F = \{0, 1, ..., k-1\}$ be a set of symbols and $X = \{\underline{x}_1, ..., \underline{x}_N\} \subset F^l$
- Let $A(\underline{x},\underline{y})=[a_{ij}]$, i,j=0,1,...,k-1, where a_{ij} is the number of places where \underline{x} has the i-th symbol and \underline{y} has the j-th symbol.

Example: l = 6, k = 3

$$\mathbf{x} = [0, 1, 2, 1, 2, 1]^T$$
 $\mathbf{y} = [1, 0, 2, 1, 0, 1]^T$
 $A(\mathbf{x}, \mathbf{y}) = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 2 & 0 \\ 1 & 0 & 1 \end{bmatrix}$

NOTE:
$$\sum_{i=0}^{k-1} \sum_{j=0}^{k-1} a_{ij} = l$$

- Several proximity measures can be expressed as combinations of the elements of $A(\underline{x},\underline{y})$.
 - Dissimilarity measures:
 - The Hamming distance (number of places where \underline{x} and \underline{y} differ)

$$d_H(\underline{x},\underline{y}) = \sum_{i=0}^{k-1} \sum_{\substack{j=0 \ j \neq i}}^{k-1} a_{ij}$$

- Several proximity measures can be expressed as combinations of the elements of $A(\underline{x},\underline{y})$.
 - Dissimilarity measures:
 - The Hamming distance (number of places where \underline{x} and \underline{y} differ)

$$d_{H}(\underline{x}, \underline{y}) = \sum_{i=0}^{k-1} \sum_{\substack{j=0 \ j \neq i}}^{k-1} a_{ij}$$

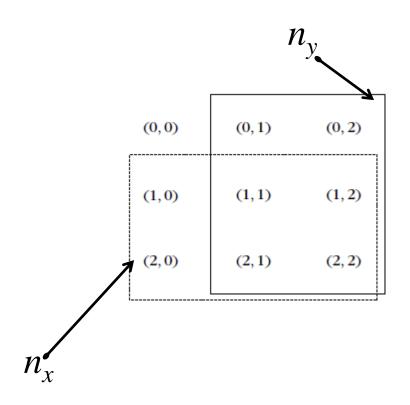
$$\boldsymbol{x} = \begin{bmatrix} 0, 1, 2, 1, 2, 1 \end{bmatrix}^{T}$$

$$\boldsymbol{y} = \begin{bmatrix} 1, 0, 2, 1, 0, 1 \end{bmatrix}^{T}$$

$$A(\boldsymbol{x}, \boldsymbol{y}) = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 2 & 0 \\ 1 & 0 & 1 \end{bmatrix}$$

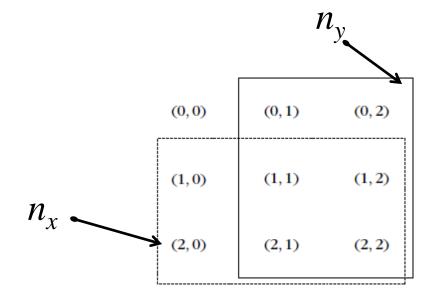
- Similarity measures:

$$A(x, y) = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 2 & 0 \\ 1 & 0 & 1 \end{bmatrix}$$



- Similarity measures:

$$A(x, y) = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 2 & 0 \\ 1 & 0 & 1 \end{bmatrix} \qquad n_x.$$



Tanimoto measure :

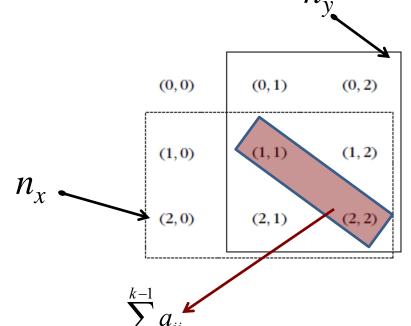
$$s_{T}(\underline{x}, \underline{y}) = \frac{\sum_{i=1}^{k-1} a_{ii}}{n_{x} + n_{y} - \sum_{i=1}^{k-1} \sum_{j=1}^{k-1} a_{ij}}$$

where

$$n_x = \sum_{i=1}^{k-1} \sum_{j=0}^{k-1} a_{ij}, \quad n_y = \sum_{i=0}^{k-1} \sum_{j=1}^{k-1} a_{ij},$$

- Similarity measures:

$$A(x, y) = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 2 & 0 \\ 1 & 0 & 1 \end{bmatrix} \qquad n_x .$$



• Tanimoto measure:

$$S_{T}(\underline{x}, \underline{y}) = \frac{\sum_{i=1}^{k-1} a_{ii}}{n_{x} + n_{y} - \sum_{i=1}^{k-1} \sum_{j=1}^{k-1} a_{ij}}$$

where

$$n_x = \sum_{i=1}^{k-1} \sum_{j=0}^{k-1} a_{ij}, \quad n_y = \sum_{i=0}^{k-1} \sum_{j=1}^{k-1} a_{ij},$$