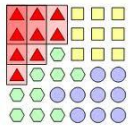
Data Mining and Data Warehousing

Unit 8

Classification and Prediction

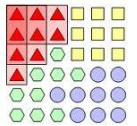
Suresh Pokharel

What is classification?



- is a data mining technique used to predict the category of categorical data by building a model based on some predictor variables (to classify data).
- Predictor variable/attribute is called class label attribute (predefined class)

What is classification?



It is a two-step process

1. Model Construction (learning step or training phase)

   - build a model to explain the target concept

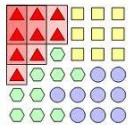
   - model is represented as classification rules, decision trees, or mathematical formulae.

2. Model Usage

   - is used for classifying future or unknown cases

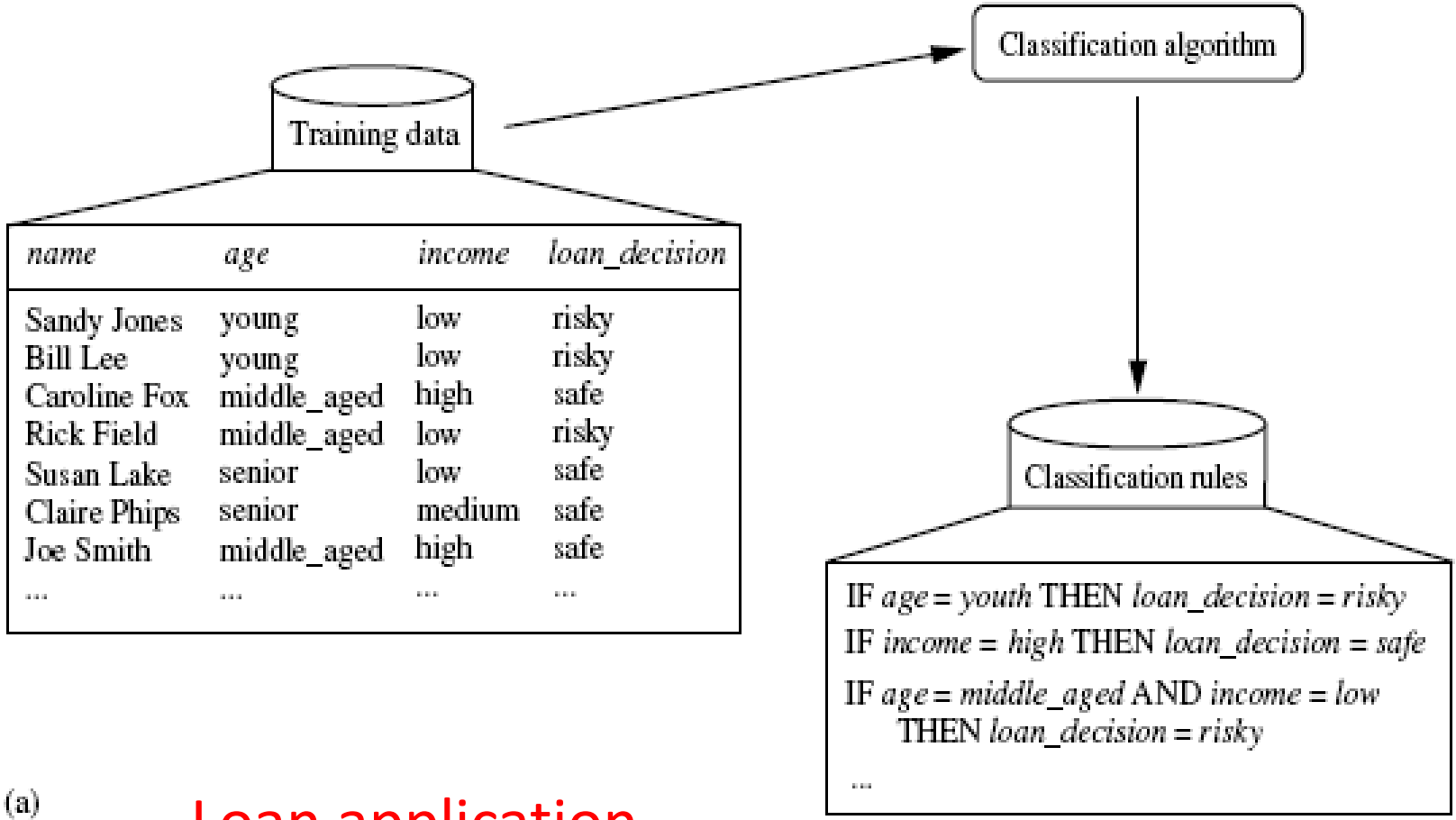
   - estimate the accuracy of the model

Example



RID	age	income	student	credit_rating	Class: buys_computer
1	youth	high	no	fair	no
2	youth	high	no	excellent	no
3	middle_aged	high	no	fair	yes
4	senior	medium	no	fair	yes
5	senior	low	yes	fair	yes
6	senior	low	yes	excellent	no
7	middle_aged	low	yes	excellent	yes
8	youth	medium	no	fair	no
9	youth	low	yes	fair	yes
10	senior	medium	yes	fair	yes
11	youth	medium	yes	excellent	yes
12	middle_aged	medium	no	excellent	yes
13	middle_aged	high	yes	fair	yes
14	senior	medium	no	excellent	no

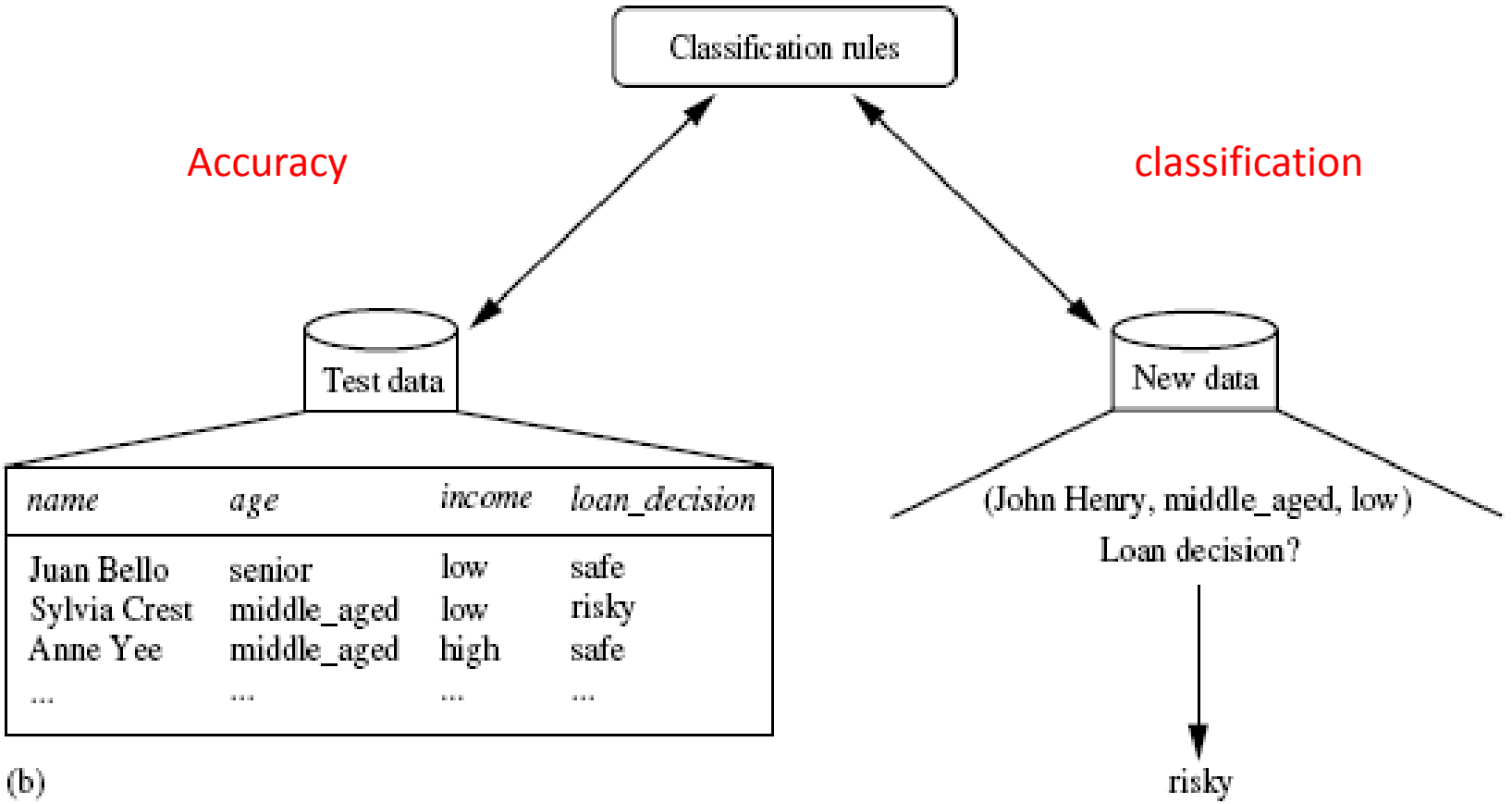
Step 1



(a)

Loan application

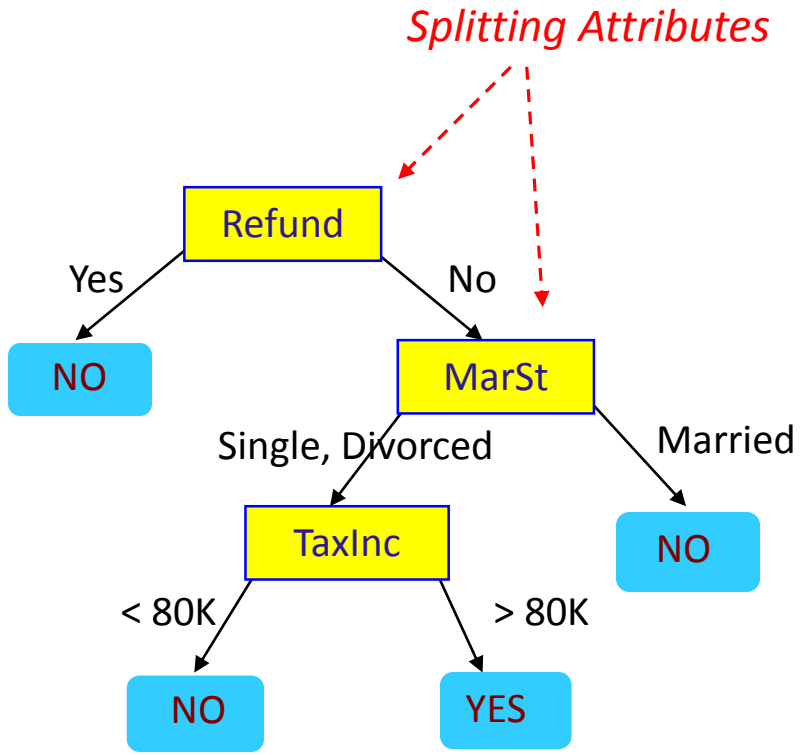
Step 2


Classification rules
Accuracy
classification
Test data
New data
name age income loan_decision
Juan Bello senior low safe
Sylvia Crest middle_aged low risky
Anne Yee middle_aged high safe
... ...
(John Henry, middle_aged, low)
Loan decision?
risky
(b)

Example of a Decision Tree

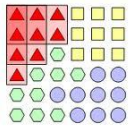
Tid	Refund	Marital Status	Taxable Income	Cheat
		categorical	continuous	class
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

Training Data



Model: Decision Tree

Another Example of Decision Tree



Tid	Refund (categorical)	Marital Status (categorical)	Taxable Income (continuous)	Cheat (class)
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
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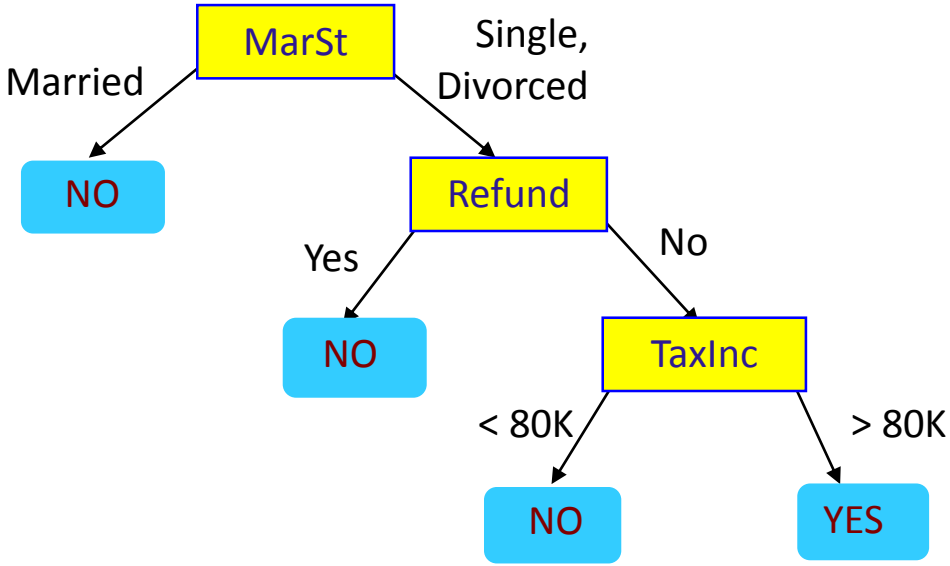


There could be more than one tree that fits the same data!

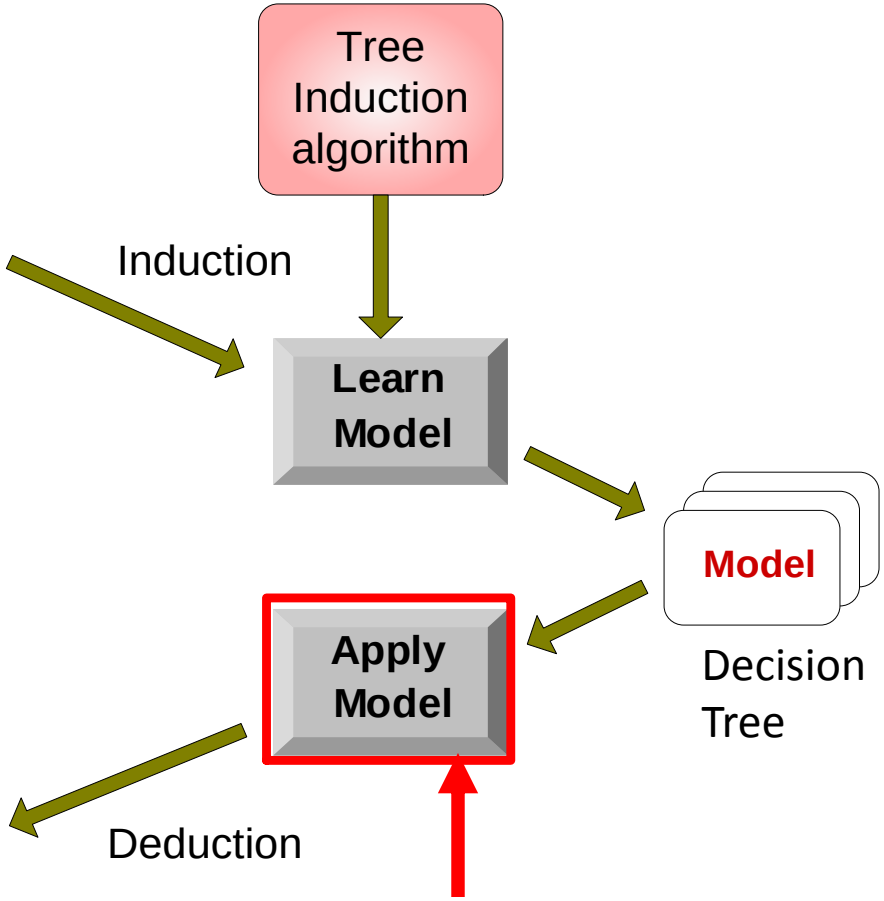
Decision Tree Classification Task

Tid	Attrib1	Attrib2	Attrib3	Class
1	Yes	Large	125K	No
2	No	Medium	100K	No
3	No	Small	70K	No
4	Yes	Medium	120K	No
5	No	Large	95K	Yes
6	No	Medium	60K	No
7	Yes	Large	220K	No
8	No	Small	85K	Yes
9	No	Medium	75K	No
10	No	Small	90K	Yes

Training Set

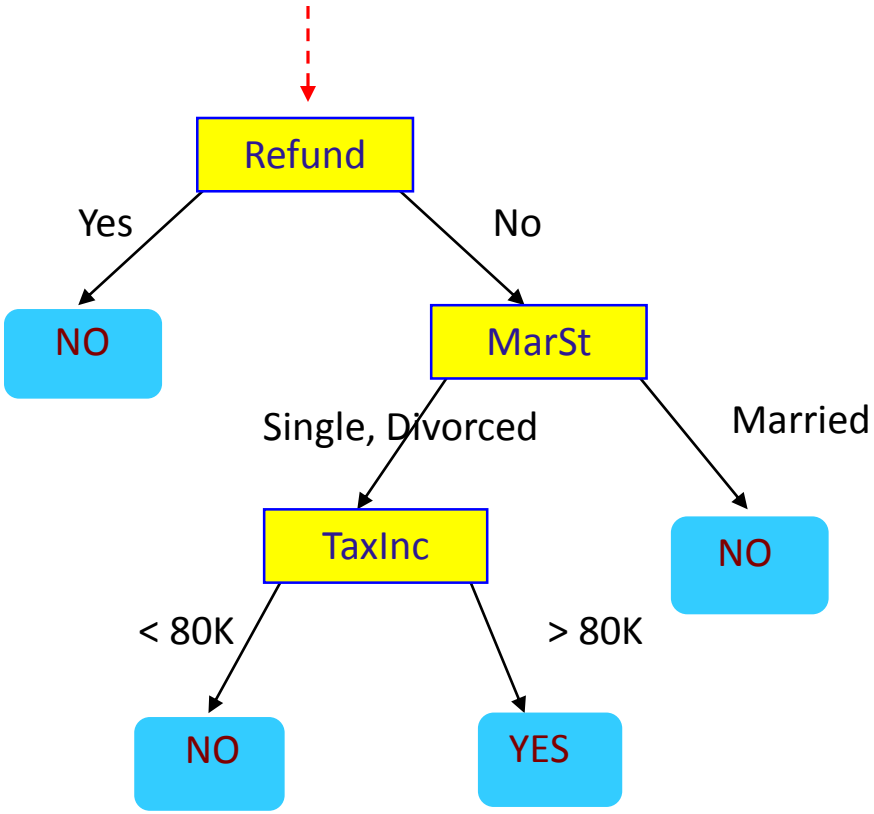
Tid	Attrib1	Attrib2	Attrib3	Class
11	No	Small	55K	?
12	Yes	Medium	80K	?
13	Yes	Large	110K	?
14	No	Small	95K	?
15	No	Large	67K	?

Test Set



Apply Model to Test Data

Start from the root of tree.



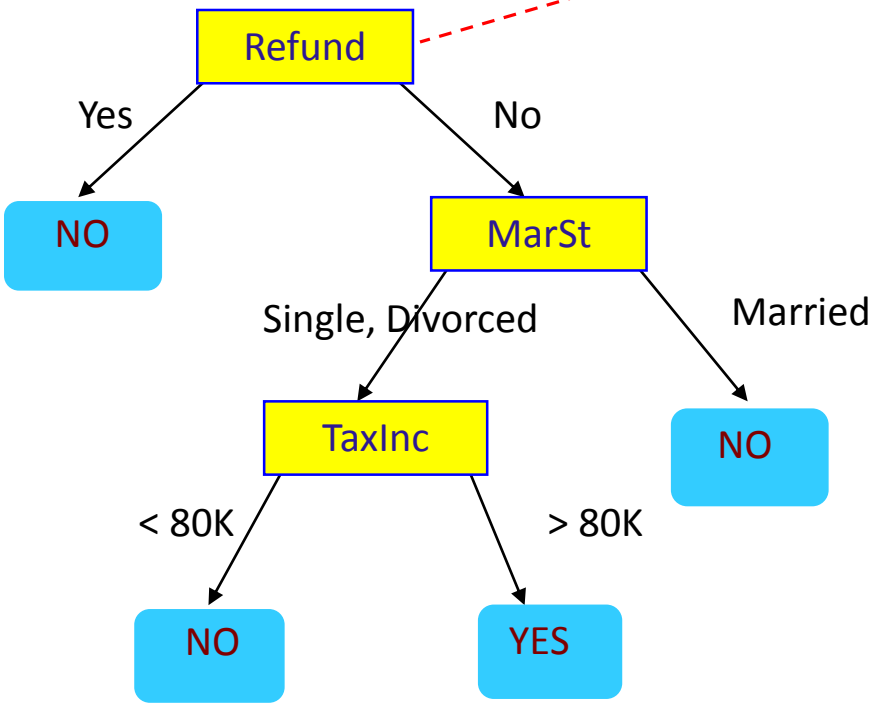
Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

Apply Model to Test Data

Test Data

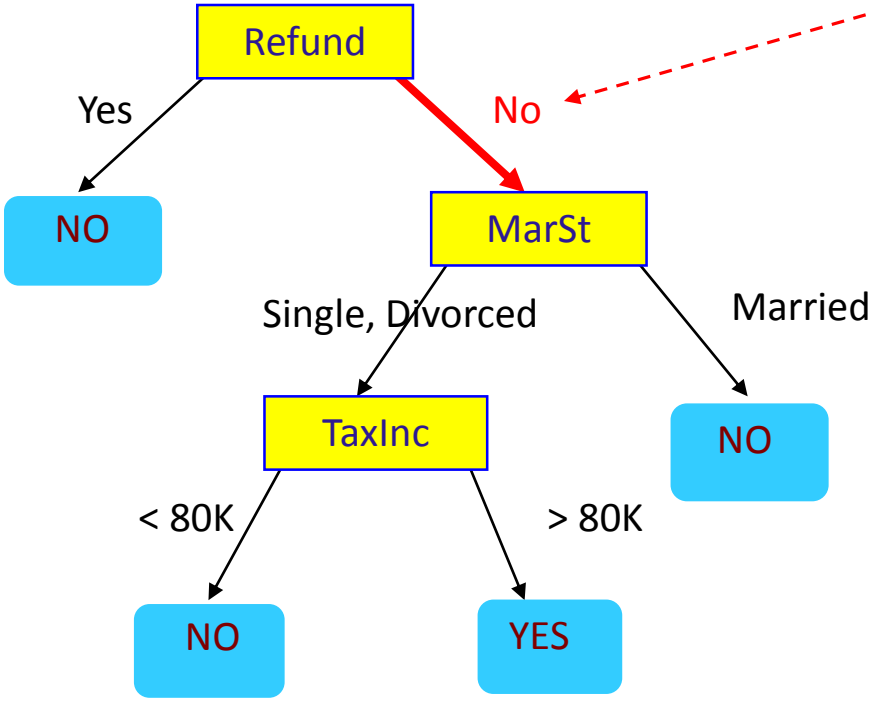
Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?



Apply Model to Test Data

Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?



Apply Model to Test Data

Test Data

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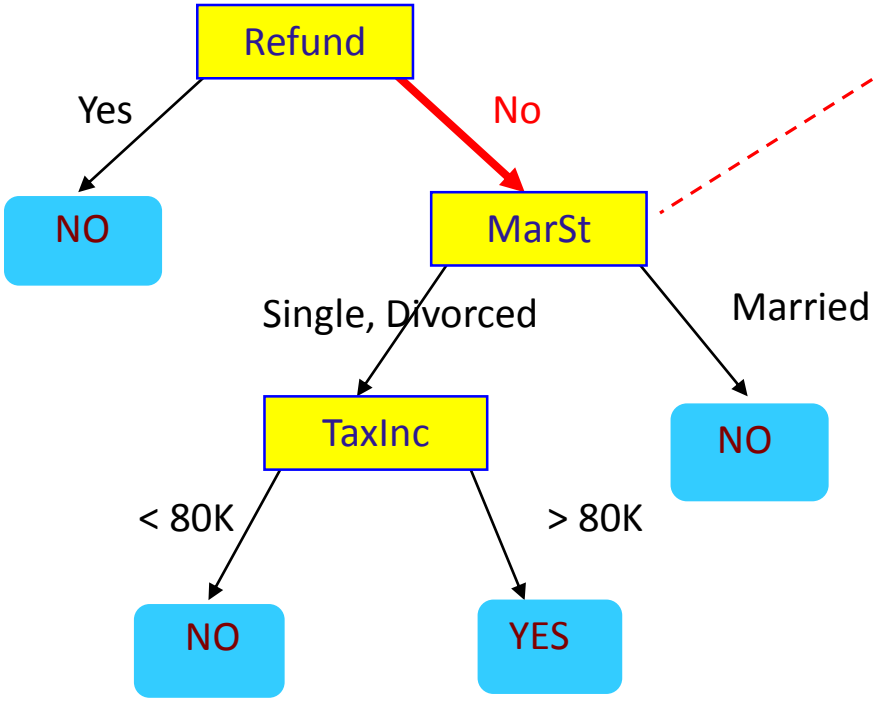
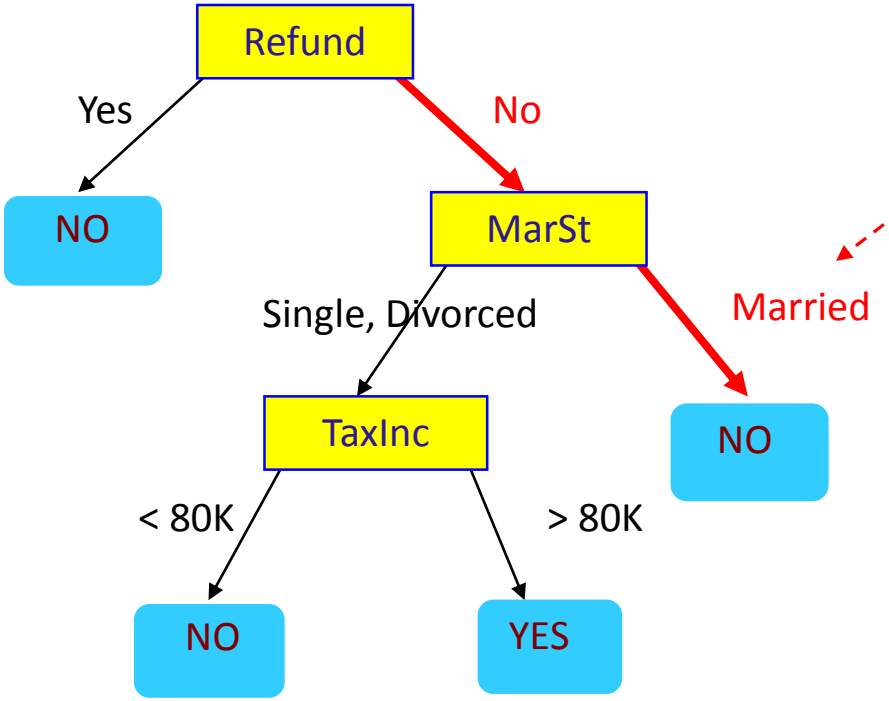
No	Married	80K	?



Apply Model to Test Data

Test Data

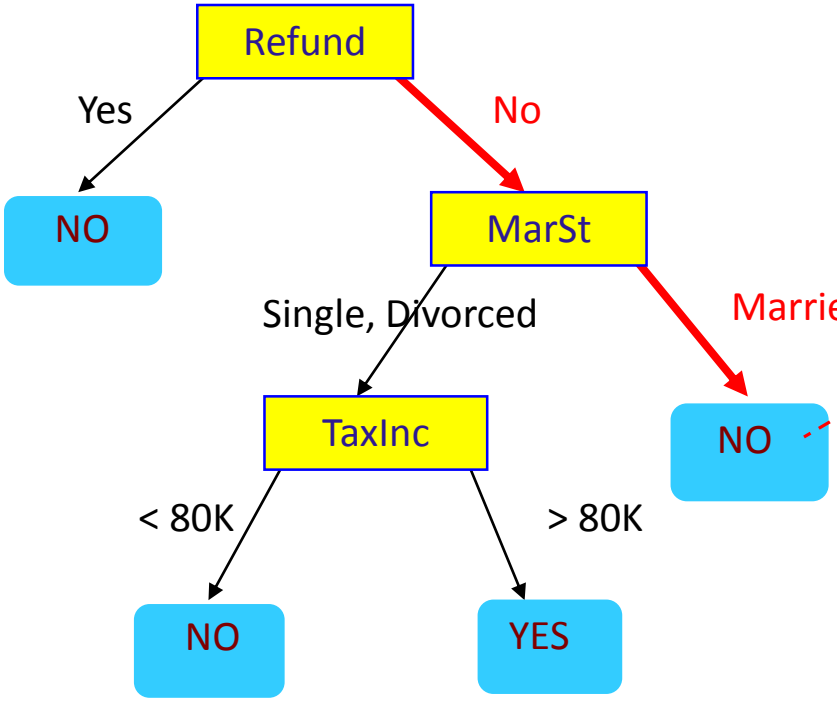
Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?



Apply Model to Test Data

Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?



Assign Cheat to “No”

Decision Tree Classification Task

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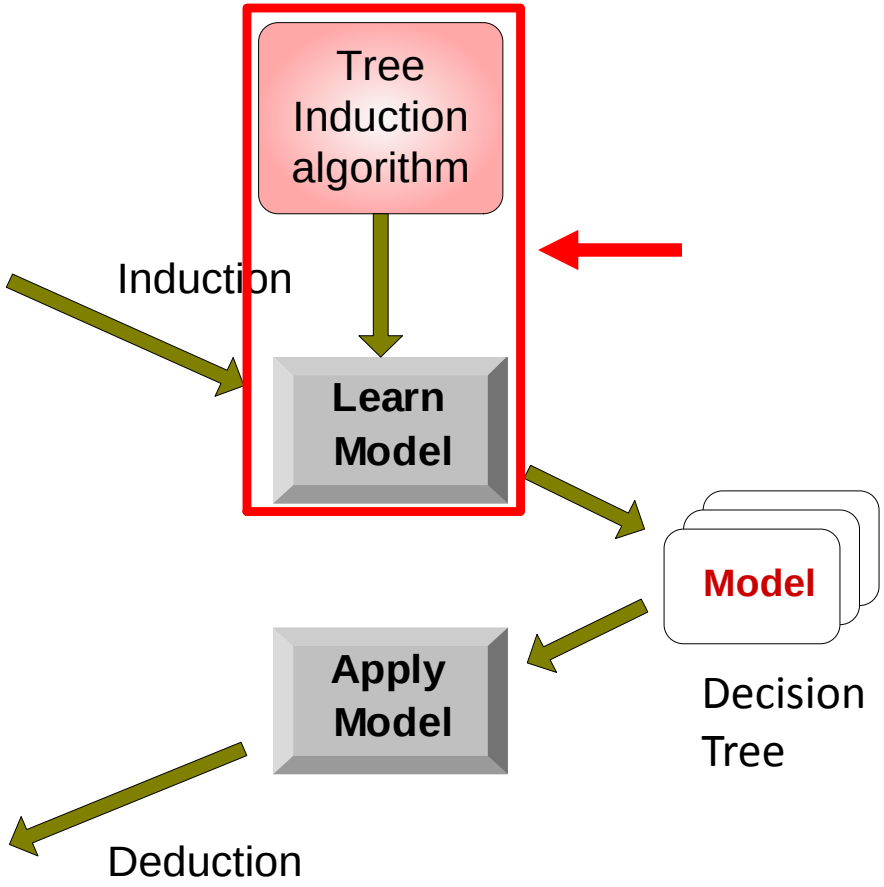
Test Set

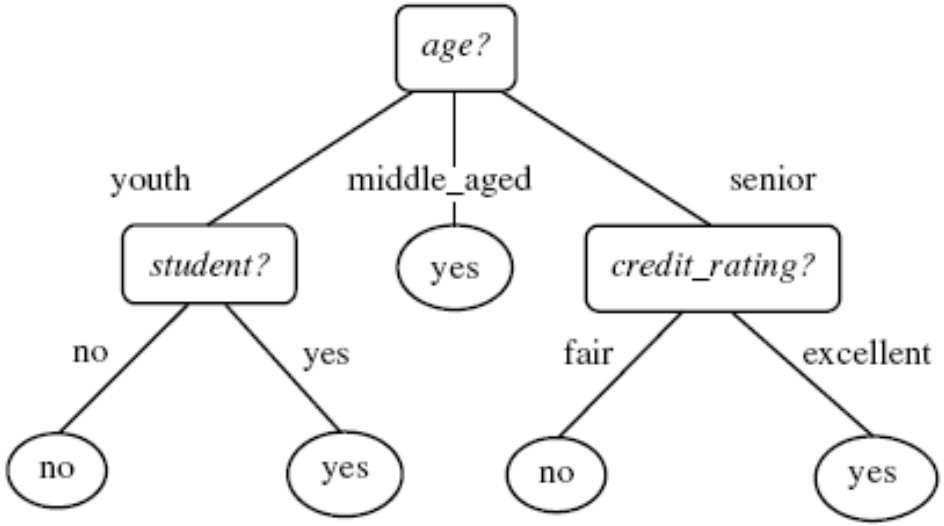


Classification by decision tree induction

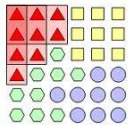
What is decision tree?

- flow chart like tree structure
- internal node denotes a test on an attribute
- each branch represents an outcome of the test
- each leaf node holds a class label

Decision tree for the concept buys computer

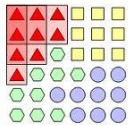


Why Decision Tree?



- Construction does not require any domain knowledge
- Can handle high dimensional data
- Learning step is simple and fast
- In general have good accuracy
- People are able to understand decision tree models after a brief explanation

Issue regarding classification & Prediction



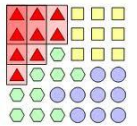
- Data Preparation

  data cleaning, relevant analysis, data transformation and reduction

- Comparing classification & prediction method

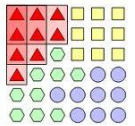
  Accuracy, speed, Robustness, scalability, interpretability

Supervised & Unsupervised Learning



- Supervised Learning (Classification)
  - Supervision: The training data are accompanied by labels indicating the class of the observations
  - New data is classified based on the training set
- Unsupervised Learning (Clustering)
  - The class labels of training data is unknown
  - Given a set of measurements, observations, etc. with the aim of establishing the existence of classes or clusters in the data

Some Decision Tree Systems



- ID3 (Quinlan 79)
- CART (Brieman et al. 84)
- Assistant (Cestnik et al. 87)
- C4.5 (Quinlan 93)
- See5 (Quinlan 97)
- ...
- Orange (Demšar, Zupan 98-03)

Decision Tree Induction- General Structure of Hunt's Algorithm

- Let D_t be the set of training records that reach a node t
- General Procedure:
  - If D_t contains records that belong the same class y_t, then t is a leaf node labeled as y_t
  - If D_t is an empty set, then t is a leaf node labeled by the default class, y_d
  - If D_t contains records that belong to more than one class, use an attribute test to split the data into smaller subsets. Recursively apply the procedure to each subset.

Tid	Refund	Marital Status	Taxable Income	Cheat
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
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7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
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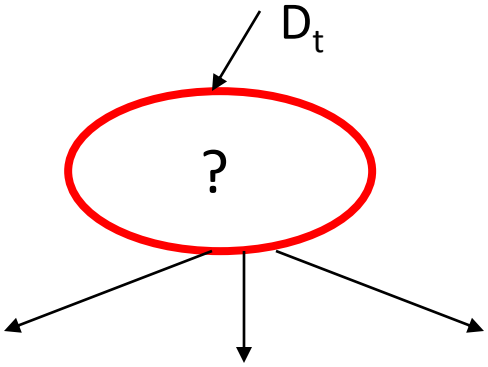
10	No	Single	90K	Yes



Decision Tree Induction- Hunt's Algorithm

Tid	Refund	Marital Status	Taxable Income	Cheat
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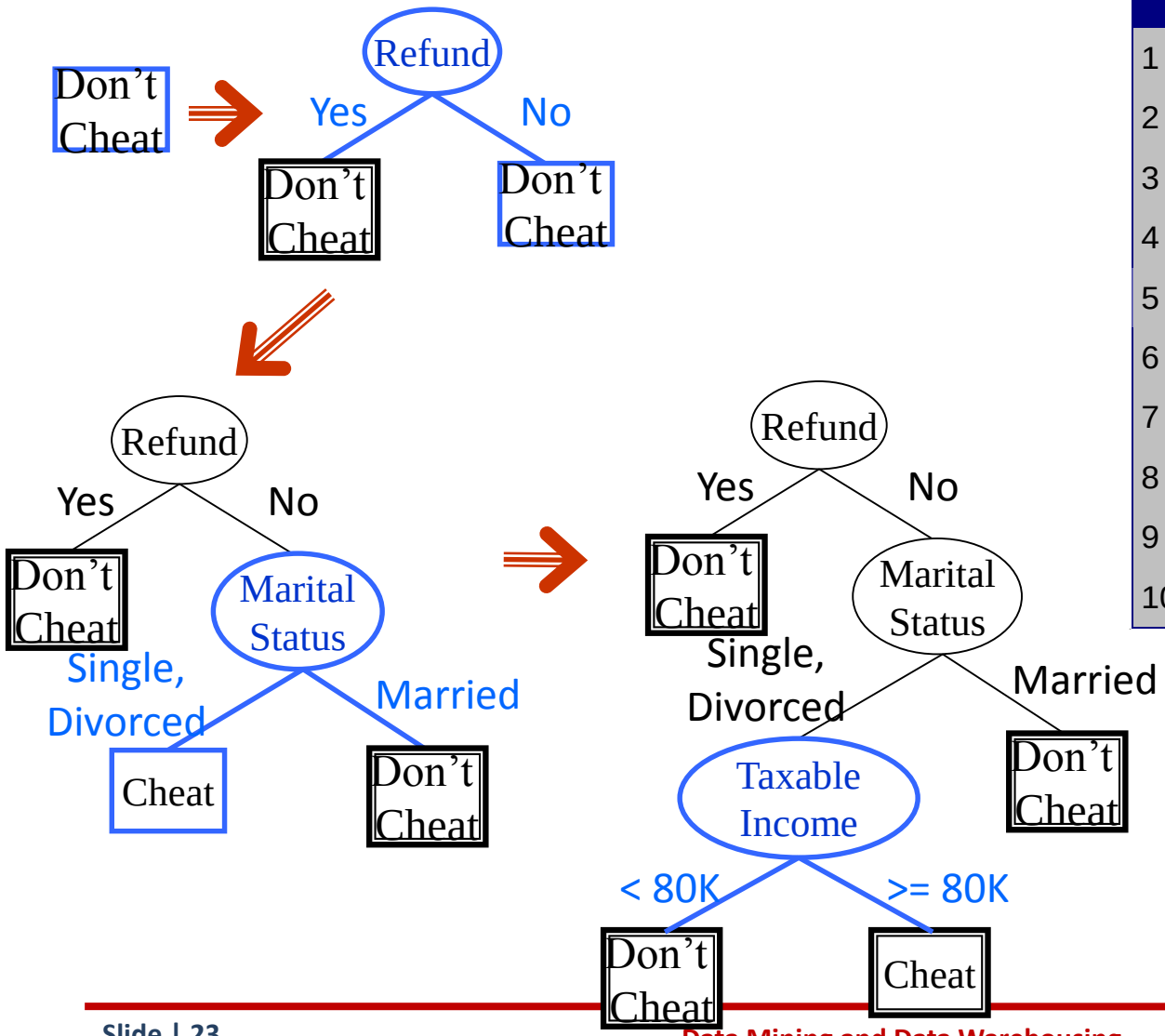
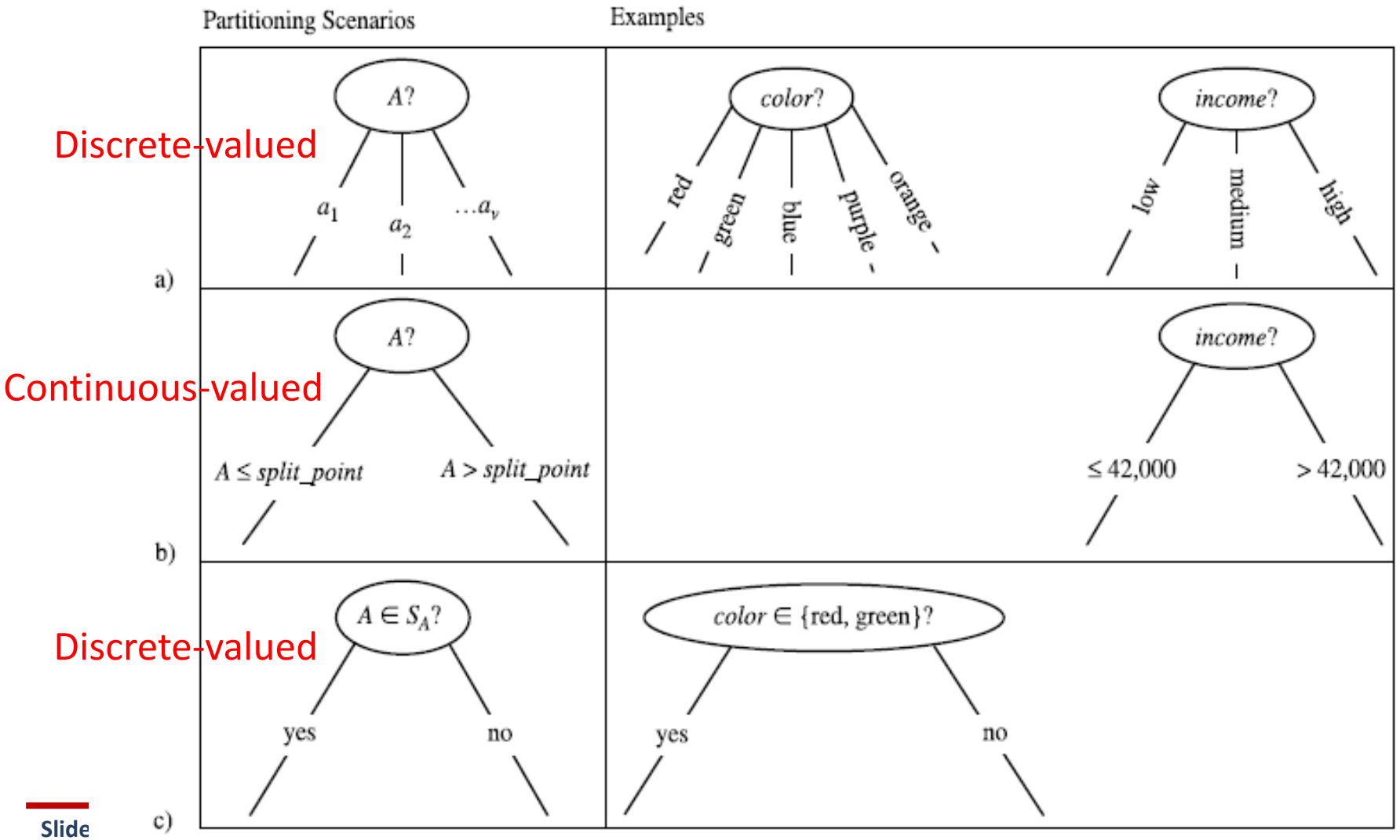


Example


Partitioning Scenarios
Examples
Discrete-valued
Continuous-valued
Discrete-valued
a)
b)
c)
A?
a_1
a_2
$\ldots a_v$
color?
red
green
blue
purple
orange
income?
low
medium
high
A?
$A \leq split\_point$
$A > split\_point$
income?
≤ 42,000
> 42,000
$A \in S_A$?
yes
no
color ∈ {red, green}?
yes
no

Attribute selection measures

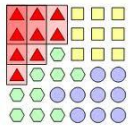
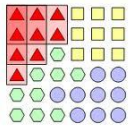


Table 6.1 Class-labeled training tuples from the *AllElectronics* customer database.

RID	*age*	*income*	*student*	*credit_rating*	*Class: buys_computer*
1	youth	high	no	fair	no
2	youth	high	no	excellent	no
3	middle_aged	high	no	fair	yes
4	senior	medium	no	fair	yes
5	senior	low	yes	fair	yes
6	senior	low	yes	excellent	no
7	middle_aged	low	yes	excellent	yes
8	youth	medium	no	fair	no
9	youth	low	yes	fair	yes
10	senior	medium	yes	fair	yes
11	youth	medium	yes	excellent	yes
12	middle_aged	medium	no	excellent	yes
13	middle_aged	high	yes	fair	yes
14	senior	medium	no	excellent	no

Information Gain, gain ratio and gini index

Attribute selection measures



- Information Gain

the expected information needed to classify a tuple in *D :* (entropy of *D)*

$$Info(D) = -\sum_{i=1}^{m} p_i \log_2(p_i),$$

- $Pi = |C_{i,D}| \,/\, |D|$
- *A* having *v* distinct values, $\{a_1, a_2, \ldots, a_v\}$
- $D_1, D_2, \ldots, D_v$

$$Info_A(D) = \sum_{j=1}^{v} \frac{|D_j|}{|D|} \times Info(D_j).$$

Attribute selection measures

$$Gain(A) = Info(D) - Info_A(D).$$ (Choose maximum value)

Table 6.1 Class-labeled training tuples from the *AllElectronics* customer database.

RID	age	income	student	credit_rating	Class: buys_computer
1	youth	high	no	fair	no
2	youth	high	no	excellent	no
3	middle_aged	high	no	fair	yes
4	senior	medium	no	fair	yes
5	senior	low	yes	fair	yes
6	senior	low	yes	excellent	no
7	middle_aged	low	yes	excellent	yes
8	youth	medium	no	fair	no
9	youth	low	yes	fair	yes
10	senior	medium	yes	fair	yes
11	youth	medium	yes	excellent	yes
12	middle_aged	medium	no	excellent	yes
13	middle_aged	high	yes	fair	yes
14	senior	medium	no	excellent	no

Example A is discrete-valued

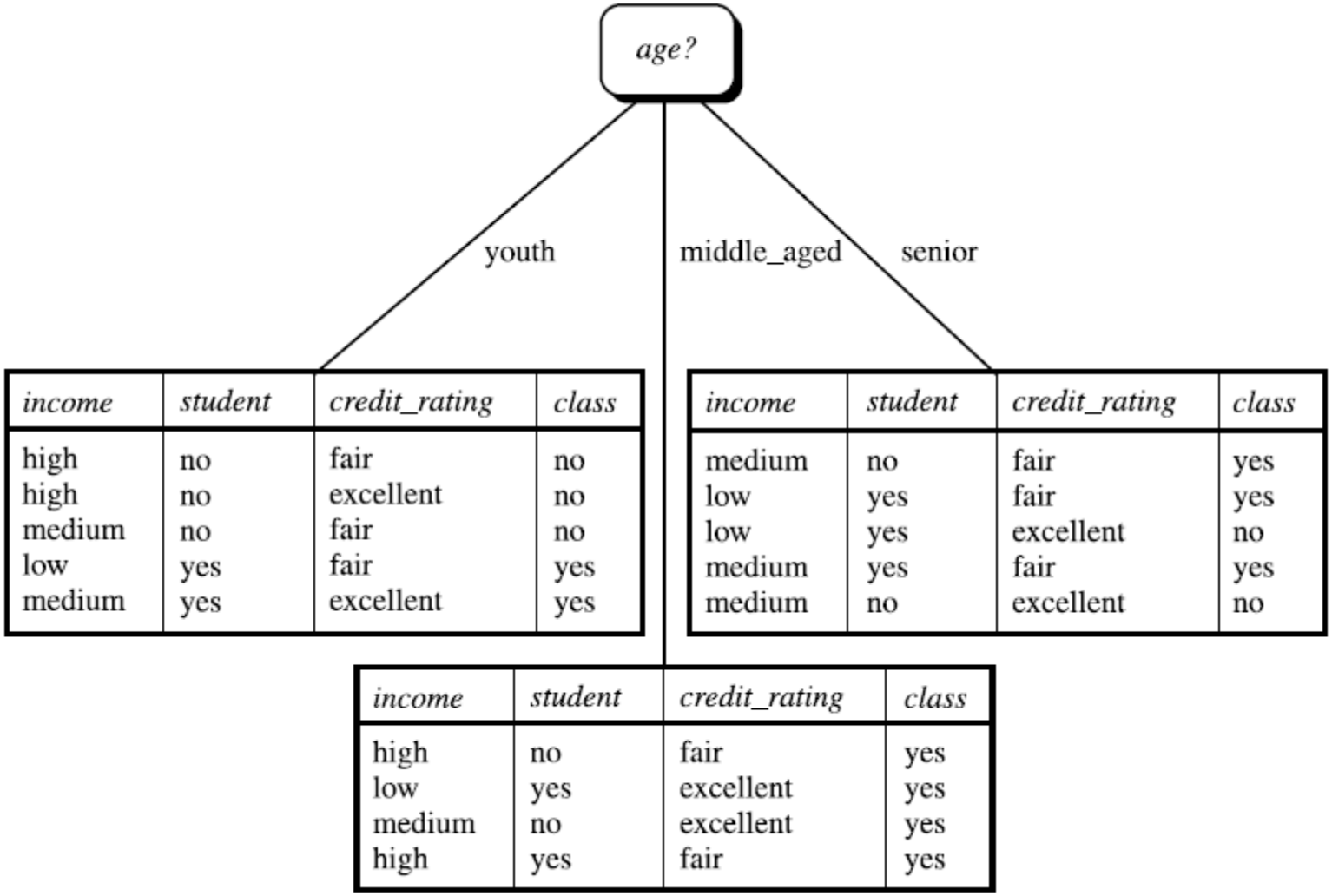
$$Info(D) = -\frac{9}{14}\log_2\left(\frac{9}{14}\right) - \frac{5}{14}\log_2\left(\frac{5}{14}\right) = 0.940 \text{ bits.}$$

$$\begin{aligned} Info_{age}(D) = & \frac{5}{14} \times \left(-\frac{2}{5}\log_2\frac{2}{5} - \frac{3}{5}\log_2\frac{3}{5}\right) \\ & + \frac{4}{14} \times \left(-\frac{4}{4}\log_2\frac{4}{4} - \frac{0}{4}\log_2\frac{0}{4}\right) \\ & + \frac{5}{14} \times \left(-\frac{3}{5}\log_2\frac{3}{5} - \frac{2}{5}\log_2\frac{2}{5}\right) \\ = & 0.694 \text{ bits.} \end{aligned}$$

$$Gain(age) = Info(D) - Info_{age}(D) = 0.940 - 0.694 = 0.246 \text{ bits.}$$

Gain(income)=0.029, Gain(student)=0.151,
Gain(credit_rating)=0.048

➔Age

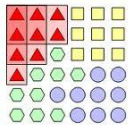


income	*student*	*credit_rating*	*class*
high	no	fair	no
high	no	excellent	no
medium	no	fair	no
low	yes	fair	yes
medium	yes	excellent	yes

income	*student*	*credit_rating*	*class*
medium	no	fair	yes
low	yes	fair	yes
low	yes	excellent	no
medium	yes	fair	yes
medium	no	excellent	no

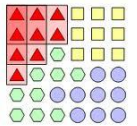
income	*student*	*credit_rating*	*class*
high	no	fair	yes
low	yes	excellent	yes
medium	no	excellent	yes
high	yes	fair	yes

What is Prediction?



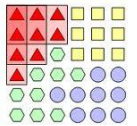
- Models continuous-valued functions, i.e. predicts unknown or missing values (numeric)
- Lost terminology of "class label attribute", instead we use "predicted attribute"
- Viewed as a mapping or function $y = f(X)$
- Example: predict the amount (in dollars) that would be safe for the bank to loan an application

What Is Prediction?



- (Numerical) prediction is similar to classification
  - construct a model
  - use model to predict continuous or ordered value for a given input
- Prediction is different from classification
  - Classification refers to predict categorical class label
  - Prediction models continuous-valued functions
- Major method for prediction: regression
  - model the relationship between one or more *independent* or **predictor** variables and a *dependent* or **response** variable
- Regression analysis
  - Linear and multiple regression
  - Non-linear regression
  - Other regression methods: generalized linear model, Poisson regression, log-linear models, regression trees

Linear Regression



- Linear regression: involves a response variable y and a single predictor variable x

  $y = w_0 + w_1 x$

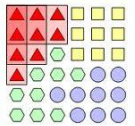
  where w_0 (y-intercept) and w_1 (slope) are regression coefficients

- Method of least squares: estimates the best-fitting straight line

$$w_1 = \frac{\sum_{i=1}^{|D|}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{|D|}(x_i - \bar{x})^2} \qquad w_0 = \bar{y} - w_1 \bar{x}$$

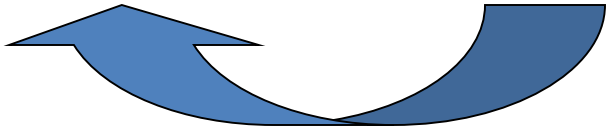
- Multiple linear regression: involves more than one predictor variable
  - Training data is of the form $(\mathbf{X_1}, y_1)$, $(\mathbf{X_2}, y_2)$,…, $(\mathbf{X_{|D|}}, y_{|D|})$
  - Ex. For 2-D data, we may have: $y = w_0 + w_1 x_1 + w_2 x_2$
  - Solvable by extension of least square method or using SAS, S-Plus
  - Many nonlinear functions can be transformed into the above

Linear Regression



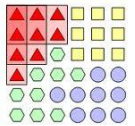
A regression model is comprised of a dependent, or response, variable and an independent, or predictor, variable.

Dependent Variable = Independent Variable(s)



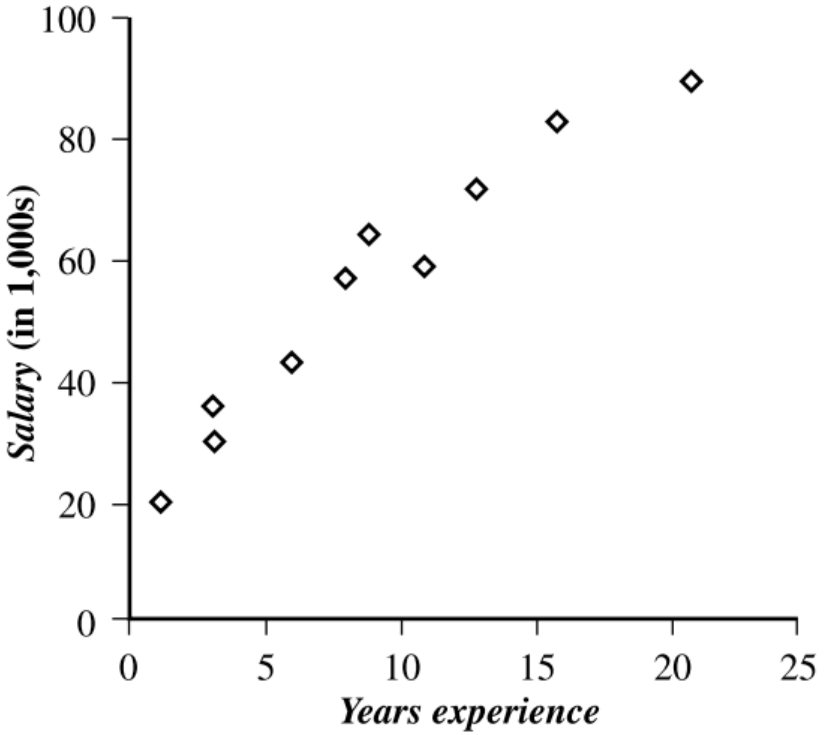
Prediction Relationship

Linear Regression



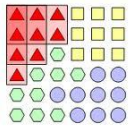
Salary data.

x years experience	*y salary (in $1000s)*
3	30
8	57
9	64
13	72
3	36
6	43
11	59
21	90
1	20
16	83



Plot of data: Although the points do not fall on a straight line, the overall pattern suggests a linear relationship between x(years experience) and y (salary)

Linear Regression



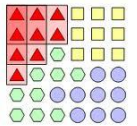
Given the above data, we compute $\bar{x} = 9.1$ and $\bar{y} = 55.4$. Substituting these values into Equations (6.50) and (6.51), we get

$$w_1 = \frac{(3-9.1)(30-55.4)+(8-9.1)(57-55.4)+\cdots+(16-9.1)(83-55.4)}{(3-9.1)^2+(8-9.1)^2+\cdots+(16-9.1)^2} = 3.5$$

$$w_0 = 55.4-(3.5)(9.1) = 23.6$$

Thus, the equation of the least squares line is estimated by $y = 23.6 + 3.5x$. Using this equation, we can predict that the salary of a college graduate with, say, 10 years of experience is \$58,600. ■

Nonlinear Regression



- Some nonlinear models can be modeled by a polynomial function
- A polynomial regression model can be transformed into linear regression model. For example,

$$y = w_0 + w_1 x + w_2 x^2 + w_3 x^3$$

convertible to linear with new variables: $x_2 = x^2$, $x_3 = x^3$

$$y = w_0 + w_1 x + w_2 x_2 + w_3 x_3$$

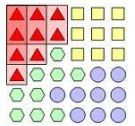
- Which is easily solved by the method of least squares using software for regression analysis
- Note that polynomial regression is a special case of multiple regression

Accuracy- Confusion Matrix

classes	buy_computer = yes	buy_computer = no	total	recognition(%)
buy_computer = yes	6954	46	7000	99.34
buy_computer = no	412	2588	3000	86.27
total	7366	2634	10000	95.42

	C_1	C_2
C_1	True positive	False negative
C_2	False positive	True negative

Classifier Accuracy

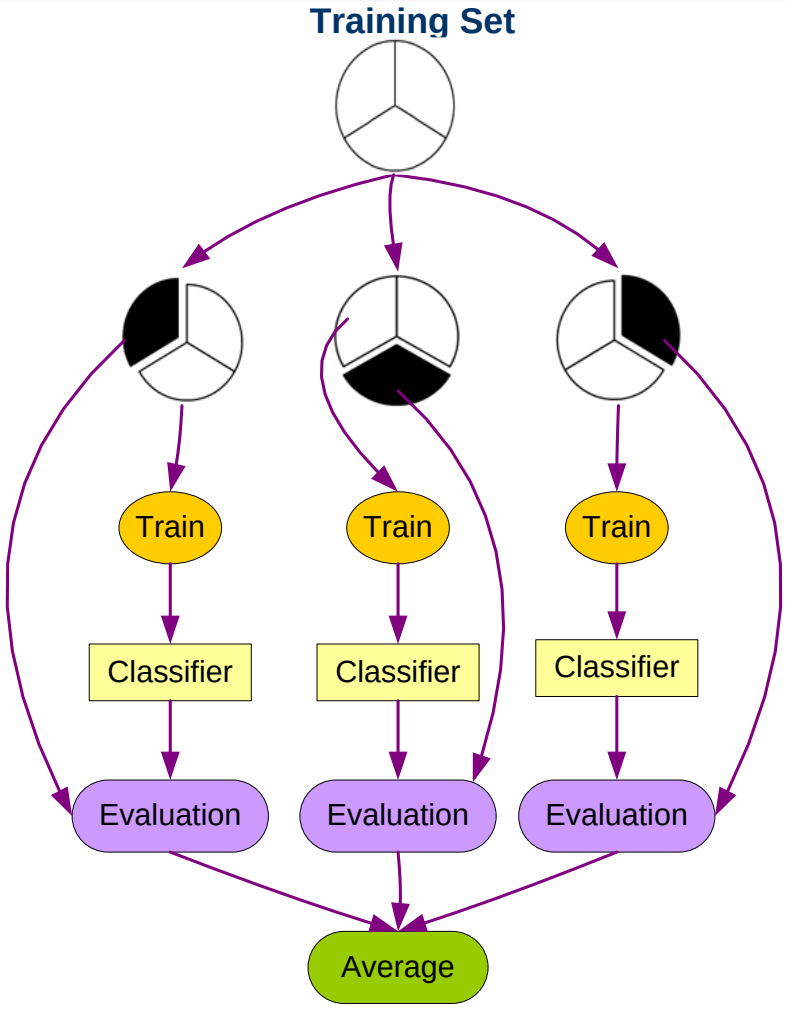


$$\text{Precision} = \frac{tp}{tp + fp}$$

$$\text{Recall} = \frac{tp}{tp + fn}$$

- Cross-validation (*k*-fold, where k = 10 is most popular)
  - Randomly partition the data into *k mutually exclusive* subsets, each approximately equal size
  - At *i*-th iteration, use D_i as test set and others as training set
  - Leave-one-out: k folds where k = # of tuples, for small sized data

Classifier Accuracy



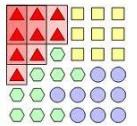
3-Crossfold Validation

Classifier Accuracy

$$\text{Precision} = \frac{tp}{tp + fp}$$

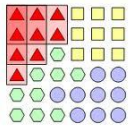
$$\text{Recall} = \frac{tp}{tp + fn}$$

What is Cluster Analysis?

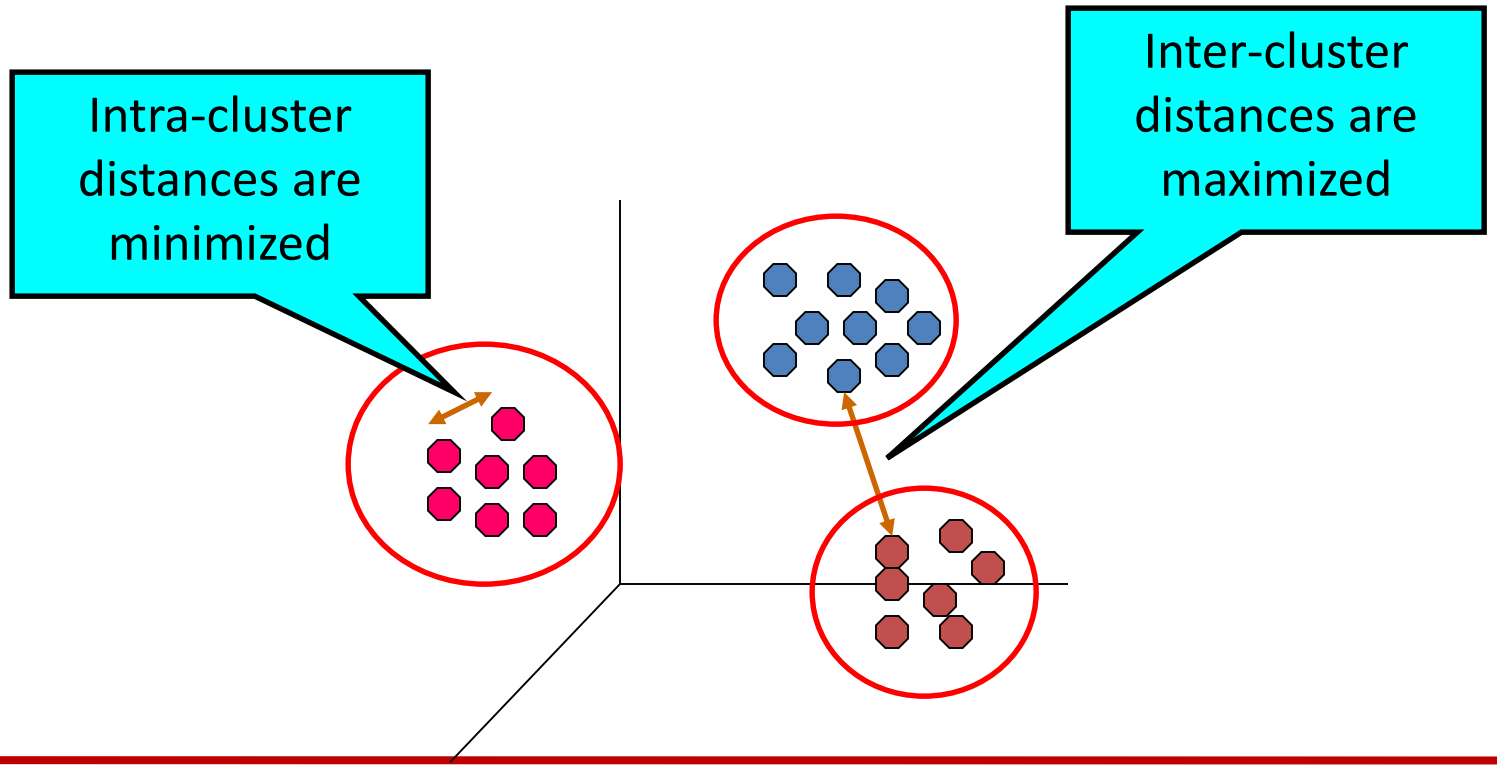


- Cluster: a collection of data objects
  - Similar to one another within the same cluster
  - Dissimilar to the objects in other clusters
- Cluster analysis
  - Grouping a set of data objects into clusters
- Clustering is unsupervised classification: no predefined classes
- Clustering is used:
  - As a stand-alone tool to get insight into data distribution
    - Visualization of clusters may unveil important information
  - As a preprocessing step for other algorithms
    - Efficient indexing or compression often relies on clustering

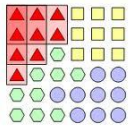
What is Cluster Analysis?



- 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

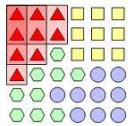


General Applications of Clustering



- Pattern Recognition
- Spatial Data Analysis
  - create thematic maps in GIS by clustering feature spaces
  - detect spatial clusters and explain them in spatial data mining
- Image Processing
  - cluster images based on their visual content
- Economic Science (especially market research)
- WWW and IR
  - document classification
  - cluster Weblog data to discover groups of similar access patterns

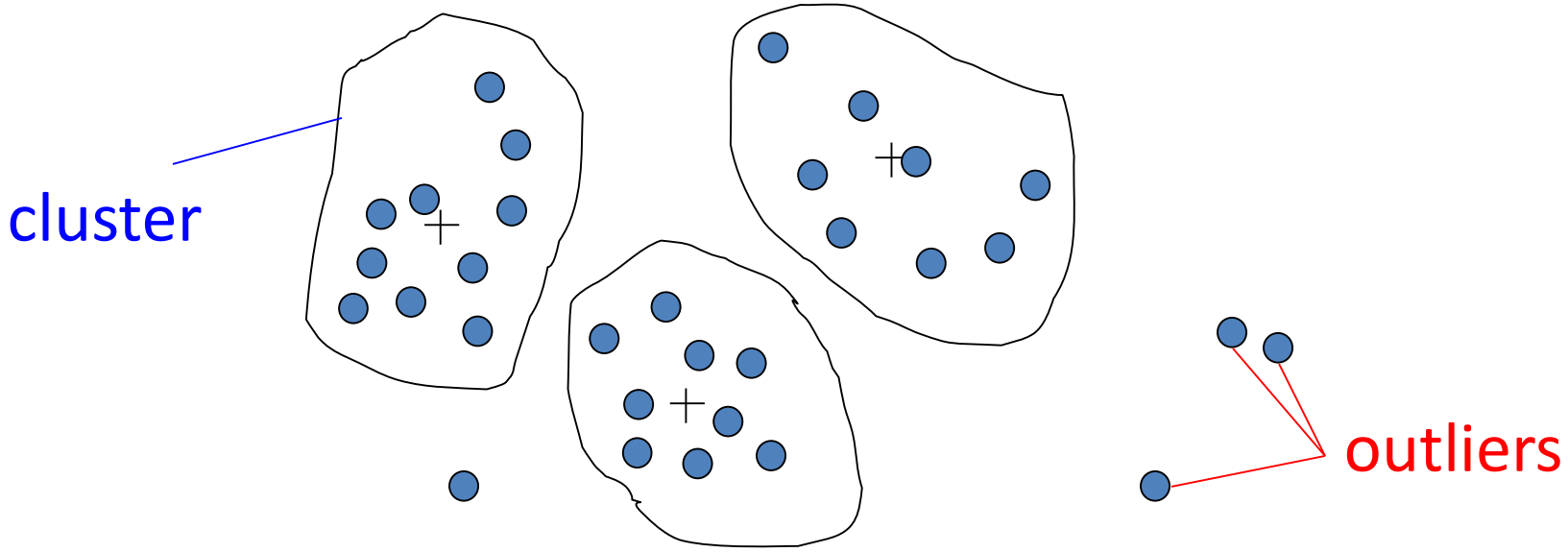
Examples of Clustering Applications



- Marketing: Help marketers discover distinct groups in their customer bases, and then use this knowledge to develop targeted marketing programs
- Land use: Identification of areas of similar land use in an earth observation database
- Insurance: Identifying groups of motor insurance policy holders with a high average claim cost
- City-planning: Identifying groups of houses according to their house type, value, and geographical location

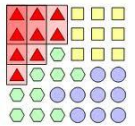
Outliers

- Outliers are objects that do not belong to any cluster or form clusters of very small cardinality



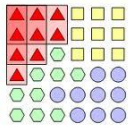
- In some applications we are interested in discovering outliers, not clusters (outlier analysis)

Major Clustering Approaches



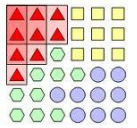
- Partitioning algorithms: Construct random partitions and then iteratively refine them by some criterion
- Hierarchical algorithms: Create a hierarchical decomposition of the set of data (or objects) using some criterion
- Density-based: based on connectivity and density functions
- Grid-based: based on a multiple-level granularity structure
- Model-based: A model is hypothesized for each of the clusters and the idea is to find the best fit of that model to each other

Partitioning Algorithms: Basic Concepts



- Partitioning method: Construct a partition of a database ***D*** of ***n*** objects into a set of ***k*** clusters
- Given a *k*, find a partition of *k clusters* that optimizes the chosen partitioning criterion
  - Global optimal: exhaustively enumerate all partitions
  - Heuristic methods: *k-means* and *k-medoids* algorithms
  - *k-means* (MacQueen'67): Each cluster is represented by the center of the cluster
  - *k-medoids* or PAM (Partition around medoids) (Kaufman & Rousseeuw'87): Each cluster is represented by one of the objects in the cluster

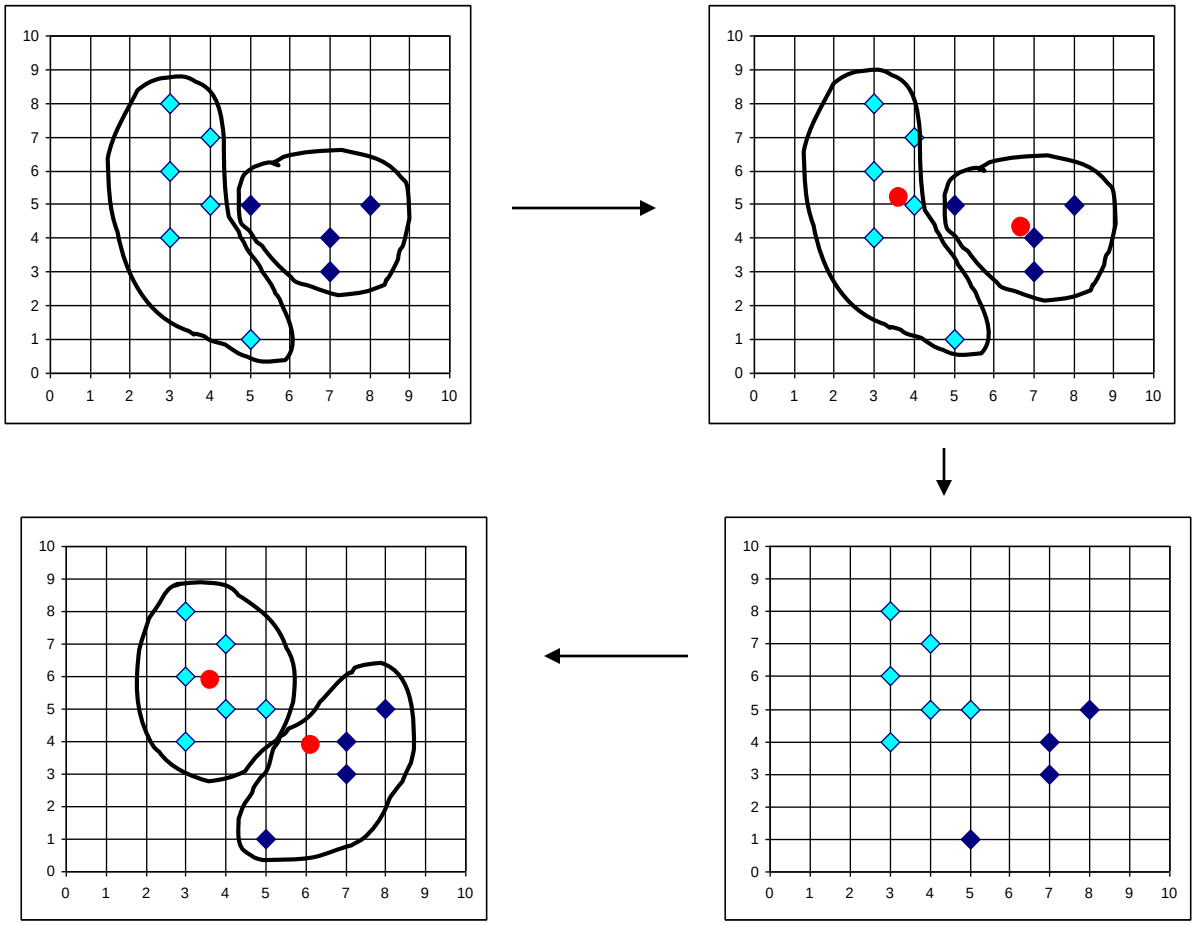
The k-means Clustering Method



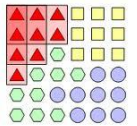
- Given *k*, the *k-means* algorithm is implemented in 4 steps:
  1. Partition objects into *k* nonempty subsets
  2. Compute seed points as the centroids of the clusters of the current partition. The centroid is the center (mean point) of the cluster.
  3. Assign each object to the cluster with the nearest seed point.
  4. Go back to Step 2, stop when no more new assignment.

The k-means Clustering Method

- Example

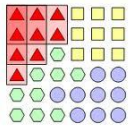


K-Means example

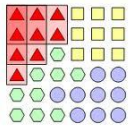


- 2, 3, 6, 8, 9, 12, 15, 18, 22 – break into 3 clusters
  - Cluster 1 - 2, 8, 15 – mean = 8.3
  - Cluster 2 - 3, 9, 18 – mean = 10
  - Cluster 3 - 6, 12, 22 – mean = 13.3
- Re-assign
  - Cluster 1 - 2, 3, 6, 8, 9 – mean = 5.6
  - Cluster 2 – mean = 0
  - Cluster 3 – 12, 15, 18, 22 – mean = 16.75
- Re-assign
  - Cluster 1 – 3, 6, 8, 9 – mean = 6.5
  - Cluster 2 – 2 – mean = 2
  - Cluster 3 = 12, 15, 18, 22 – mean = 16.75

K-Means example (continued)



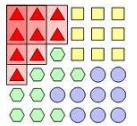
- Re-assign
  - Cluster 1 - 6, 8, 9 – mean = 7.6
  - Cluster 2 – 2, 3 – mean = 2.5
  - Cluster 3 – 12, 15, 18, 22 – mean = 16.75
- Re-assign
  - Cluster 1 - 6, 8, 9 – mean = 7.6
  - Cluster 2 – 2, 3 - mean = 2.5
  - Cluster 3 – 12, 15, 18, 22 – mean = 16.75
- No change, so we're done



K-Means example – different starting order

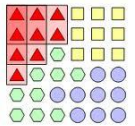
- 2, 3, 6, 8, 9, 12, 15, 18, 22 – break into 3 clusters
  - Cluster 1 - 2, 12, 18 – mean = 10.6
  - Cluster 2 - 6, 9, 22 – mean = 12.3
  - Cluster 3 – 3, 8, 15 – mean = 8.6
- Re-assign
  - Cluster 1 - mean = 0
  - Cluster 2 – 12, 15, 18, 22 - mean = 16.75
  - Cluster 3 – 2, 3, 6, 8, 9 – mean = 5.6
- Re-assign
  - Cluster 1 – 2 – mean = 2
  - Cluster 2 – 12, 15, 18, 22 – mean = 16.75
  - Cluster 3 = 3, 6, 8, 9 – mean = 6.5

K-Means example (continued)



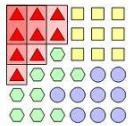
- Re-assign
  - Cluster 1 – 2, 3 – mean = 2.5
  - Cluster 2 – 12, 15, 18, 22 – mean = 16.75
  - Cluster 3 – 6, 8, 9 – mean = 7.6
- Re-assign
  - Cluster 1 – 2, 3 – mean = 2.5
  - Cluster 2 – 12, 15, 18, 22 - mean = 16.75
  - Cluster 3 – 6, 8, 9 – mean = 7.6
- No change, so we're done

Comments on the k-means Method



- Strength
  - *Relatively efficient*: $O(tkn)$, where n is # objects, k is # clusters, and t is # iterations. Normally, $k, t << n$.
- Weaknesses
  - Applicable only when *mean* is defined, then what about categorical data?
  - Need to specify *k,* the *number* of clusters, in advance
  - Unable to handle noisy data and *outliers*

K-Medoids Method

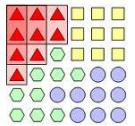


- Minimize the sensitivity of k-means to outliers
- Pick actual objects to represent clusters instead of mean values
- Each remaining object is clustered with the representative object (Medoid) to which is the most similar
- The algorithm minimizes the sum of the dissimilarities between each object and its corresponding reference point

$$E = \sum_{i-1}^{k} \sum_{p \in Ci} |\mathrm{P} - Oi|$$

E: the sum of absolute error for all objects in the data set
P: the data point in the space representing an object
Oi: is the representative object of cluster Ci

K-Medoids Method: The Idea

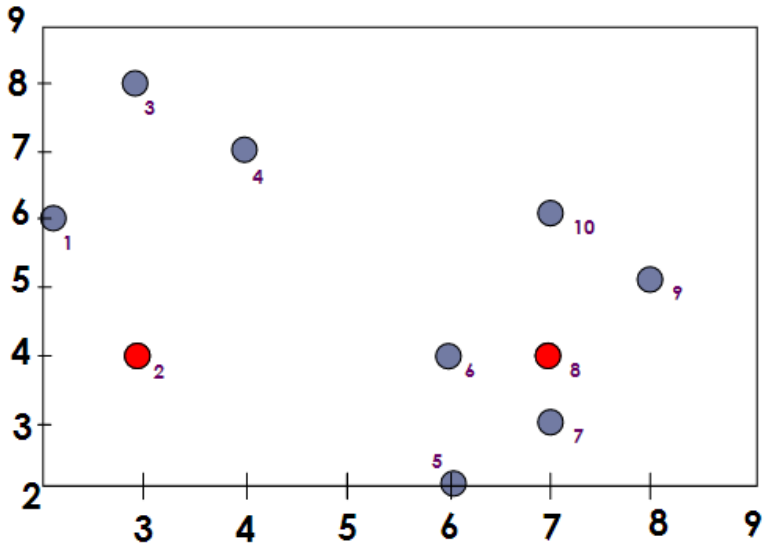


- Initial representatives are chosen randomly
- The iterative process of replacing representative objects by no representative objects continues as long as the quality of the clustering is improved
- For each representative Object O
  - For each non-representative object R, swap O and R
- Choose the configuration with the lowest cost
- Cost function is the difference in absolute error-value if a current representative object is replaced by a non-representative object

K-Medoids Method: Example

Data Objects

	A_1	A_2
O_1	2	6
O_2	3	4
O_3	3	8
O_4	4	7
O_5	6	2
O_6	6	4
O_7	7	3
O_8	7	4
O_9	8	5
O_{10}	7	6



Goal: create two clusters

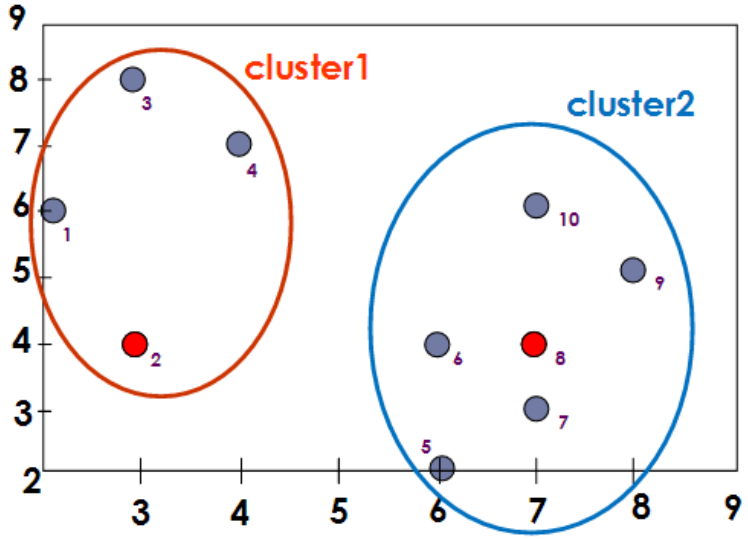
Choose randmly two medoids

$O_2 = (3,4)$
$O_8 = (7,4)$

K-Medoids Method: Example

Data Objects

	A_1	A_2
O_1	2	6
O_2	3	4
O_3	3	8
O_4	4	7
O_5	6	2
O_6	6	4
O_7	7	3
O_8	7	4
O_9	8	5
O_{10}	7	6



→Assign each object to the closest representative object

→Using L1 Metric (Manhattan), we form the following clusters

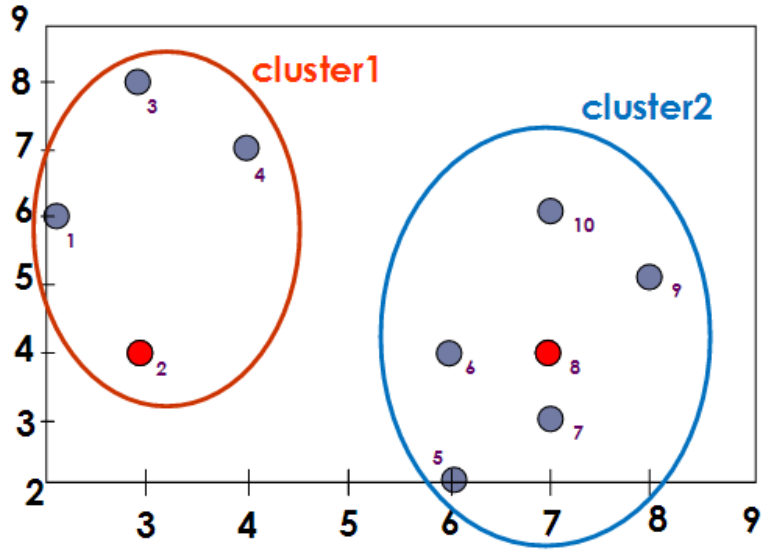
Cluster1 = $\{O_1, O_2, O_3, O_4\}$

Cluster2 = $\{O_5, O_6, O_7, O_8, O_9, O_{10}\}$

K-Medoids Method: Example

Data Objects

	A_1	A_2
O_1	2	6
O_2	3	4
O_3	3	8
O_4	4	7
O_5	6	2
O_6	6	4
O_7	7	3
O_8	7	4
O_9	8	5
O_{10}	7	6



→Compute the absolute error criterion **[for the set of Medoids (O2,O8)]**

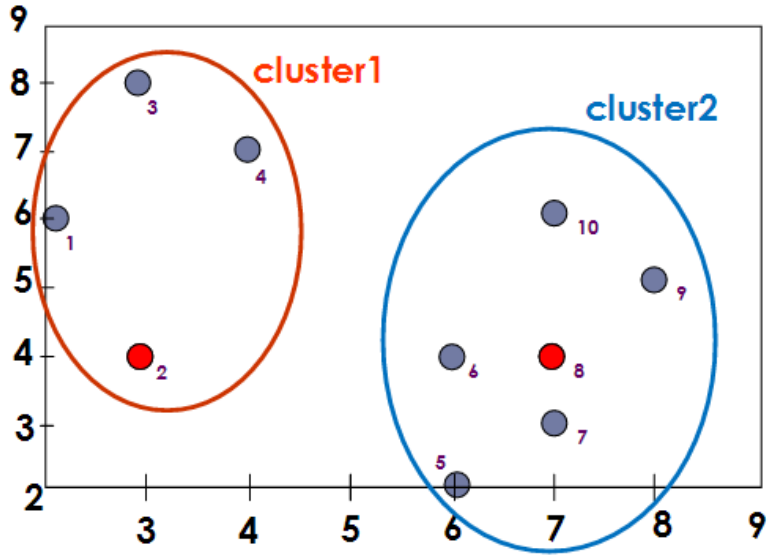
$$E=\sum_{i=1}^{k}\sum_{p\in C_i}|p-o_i| = |o_1-o_2|+|o_3-o_2|+|o_4-o_2|$$

$$+|o_5-o_8|+|o_6-o_8|+|o_7-o_8|+|o_9-o_8|+|o_{10}-o_8|$$

K-Medoids Method: Example

Data Objects

	A_1	A_2
O_1	2	6
O_2	3	4
O_3	3	8
O_4	4	7
O_5	6	2
O_6	6	4
O_7	7	3
O_8	7	4
O_9	8	5
O_{10}	7	6



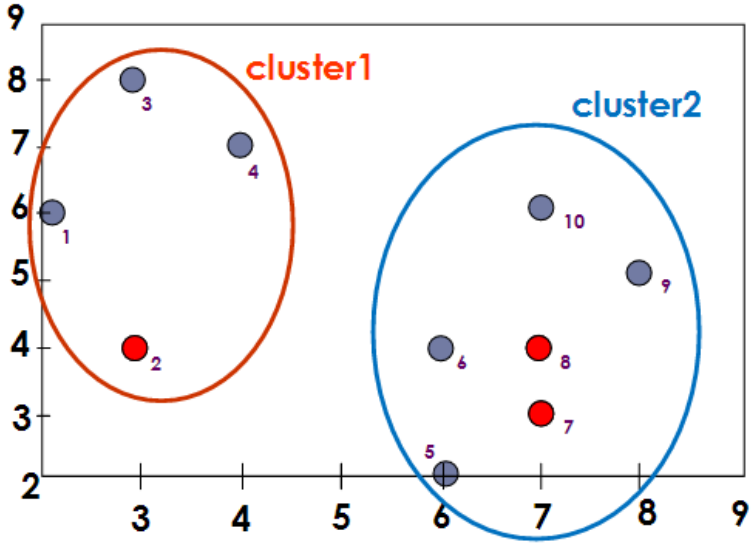
→The absolute error criterion **[for the set of Medoids (O2,O8)]**

$$E = (3+4+4)+(3+1+1+2+2) = 20$$

K-Medoids Method: Example

Data Objects

	A_1	A_2
O_1	2	6
O_2	3	4
O_3	3	8
O_4	4	7
O_5	6	2
O_6	6	4
O_7	7	3
O_8	7	4
O_9	8	5
O_{10}	7	6



→Choose a random object O_7

→Swap O8 and O7

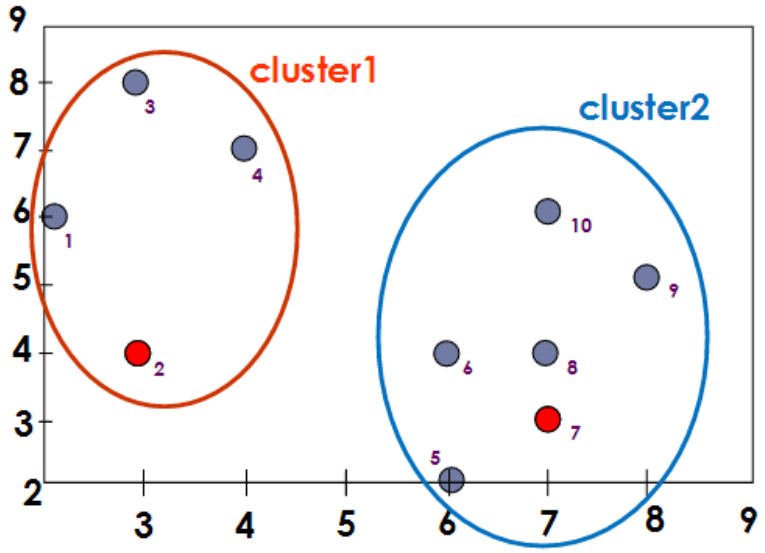
→Compute the absolute error criterion **[for the set of Medoids (O2,O7)]**

$$E = (3+4+4)+(2+2+1+3+3) = 22$$

K-Medoids Method: Example

Data Objects

	A_1	A_2
O_1	2	6
O_2	3	4
O_3	3	8
O_4	4	7
O_5	6	2
O_6	6	4
O_7	7	3
O_8	7	4
O_9	8	5
O_{10}	7	6



→Compute the cost function

Absolute error [for O_2, O_7] – Absolute error [O_2, O_8]

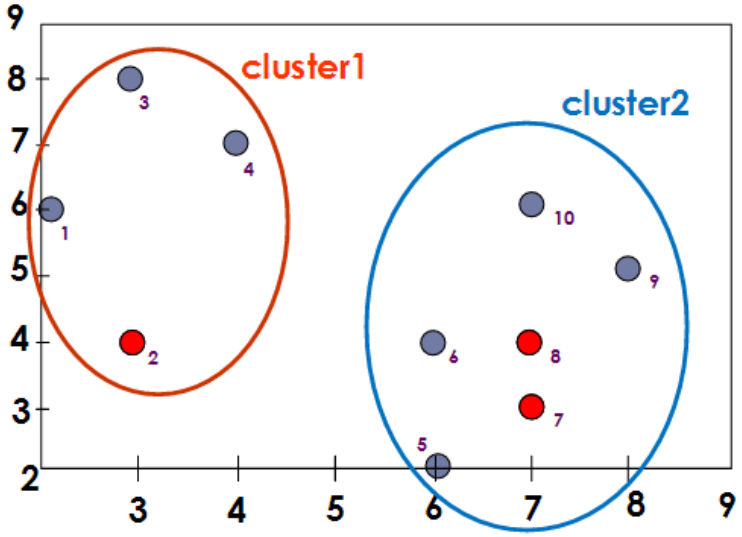
$$S = 22 - 20$$

S> 0 ⇒ it is a bad idea to replace O_8 by O_7

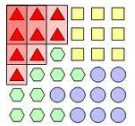
K-Medoids Method: Example

Data Objects

	A_1	A_2
O_1	2	6
O_2	3	4
O_3	3	8
O_4	4	7
O_5	6	2
O_6	6	4
O_7	7	3
O_8	7	4
O_9	8	5
O_{10}	7	6



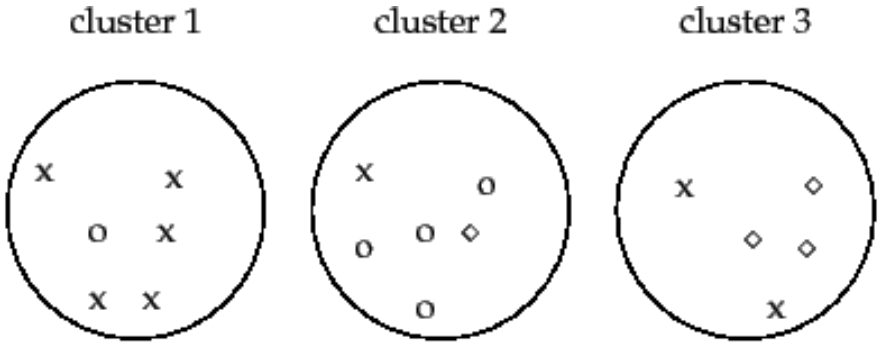
- In this example, changing the medoid of cluster 2 did not change the assignments of objects to clusters.
- What are the possible cases when we replace a medoid by another object?



Validation Criteria : Clustering

- Purity
- *Rand index*
- *F measure*

Clustering: Purity

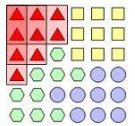


► **Figure 16.1** Purity as an external evaluation criterion for cluster quality. Majority class and number of members of the majority class for the three clusters are: x, 5 (cluster 1); o, 4 (cluster 2); and ⋄, 3 (cluster 3). Purity is $(1/17) \times (5+4+3) \approx 0.71$.

$$\text{purity}(\Omega, \mathbb{C}) = \frac{1}{N} \sum_k \max_j |\omega_k \cap c_j|$$

where $\Omega = \{\omega_1, \omega_2, \ldots, \omega_K\}$ is the set of cluster and $\mathbb{C} = \{c_1, c_2, \ldots, c_J\}$ is the set of classes

High purity is easy to achieve when the number of clusters is large - in particular, purity is 1 if each document gets its own cluster. Thus, we cannot use purity to trade off the quality of the clustering against the number of clusters.



Clustering: Rand Index

A true positive (TP) decision assigns two similar documents to the same cluster, a true negative (TN) decision assigns two dissimilar documents to different clusters. There are two types of errors we can commit. A (FP) decision assigns two dissimilar documents to the same cluster. A (FN) decision assigns two similar documents to different clusters. The *Rand index* ( ) measures the percentage of decisions that are correct.

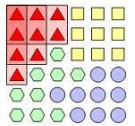
$$\mathrm{RI} = \frac{\mathrm{TP} + \mathrm{TN}}{\mathrm{TP} + \mathrm{FP} + \mathrm{FN} + \mathrm{TN}}$$

$$\mathrm{TP} + \mathrm{FP} = \binom{6}{2} + \binom{6}{2} + \binom{5}{2} = 40$$

$$\mathrm{TP} = \binom{5}{2} + \binom{4}{2} + \binom{3}{2} + \binom{2}{2} = 20$$

$$\mathrm{FP} = 40 - 20 = 20$$

Clustering: Rand Index



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

RI is then $(20 + 72)/(20 + 20 + 24 + 72) \approx 0.68$.

Clustering: F-Measure

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

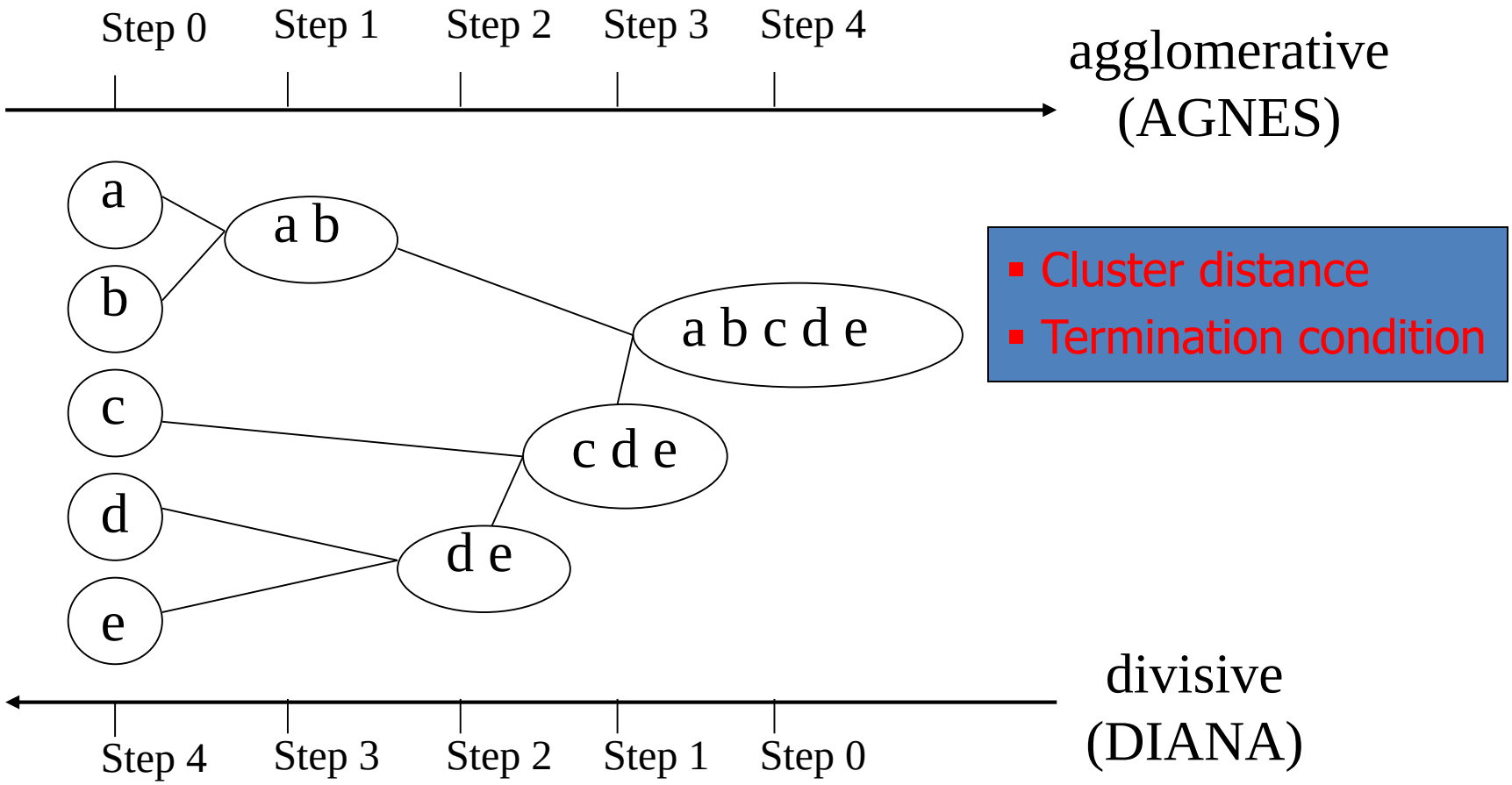
$$P = \frac{\text{TP}}{\text{TP} + \text{FP}} \qquad R = \frac{\text{TP}}{\text{TP} + \text{FN}} \qquad F_\beta = \frac{(\beta^2 + 1)PR}{\beta^2 P + R}$$

$$P = 20/40 = 0.5 \qquad R = 20/44 \approx 0.455 \qquad F_1 \approx 0.48 \qquad \beta = 1$$

$$F_5 \approx 0.456 \qquad \beta = 5$$

In information retrieval, evaluating clustering with F has the advantage that the measure is already familiar to the research community.

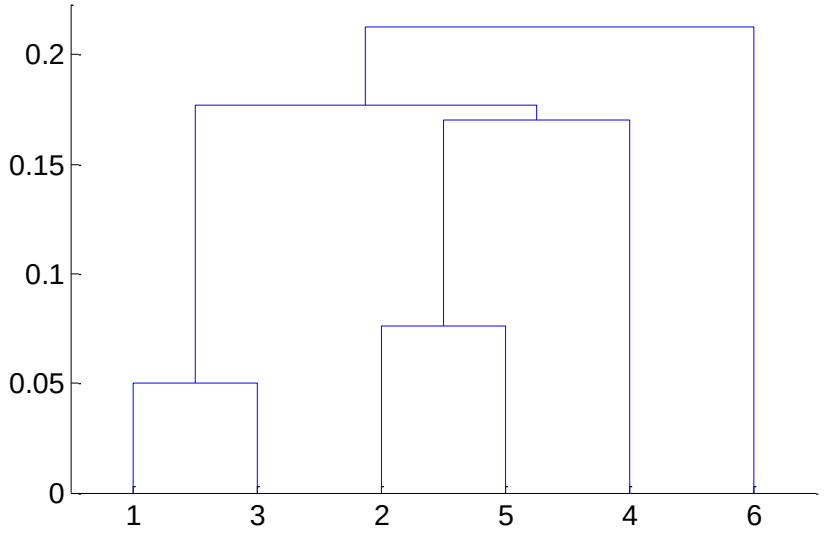
Hierarchical Clustering

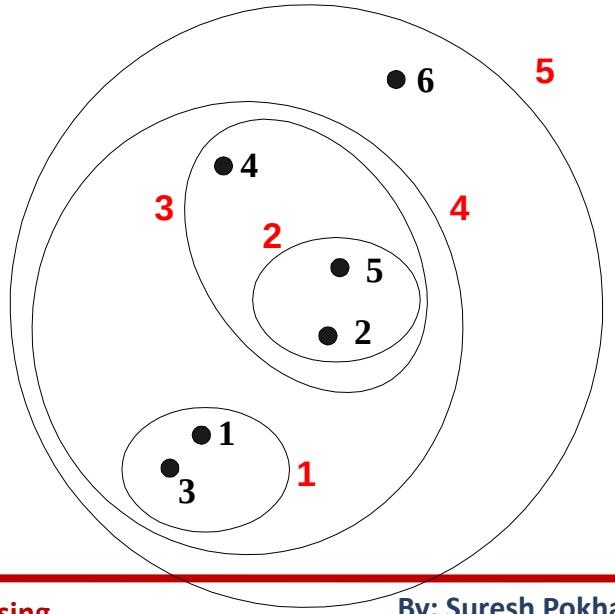


- Cluster distance
- Termination condition

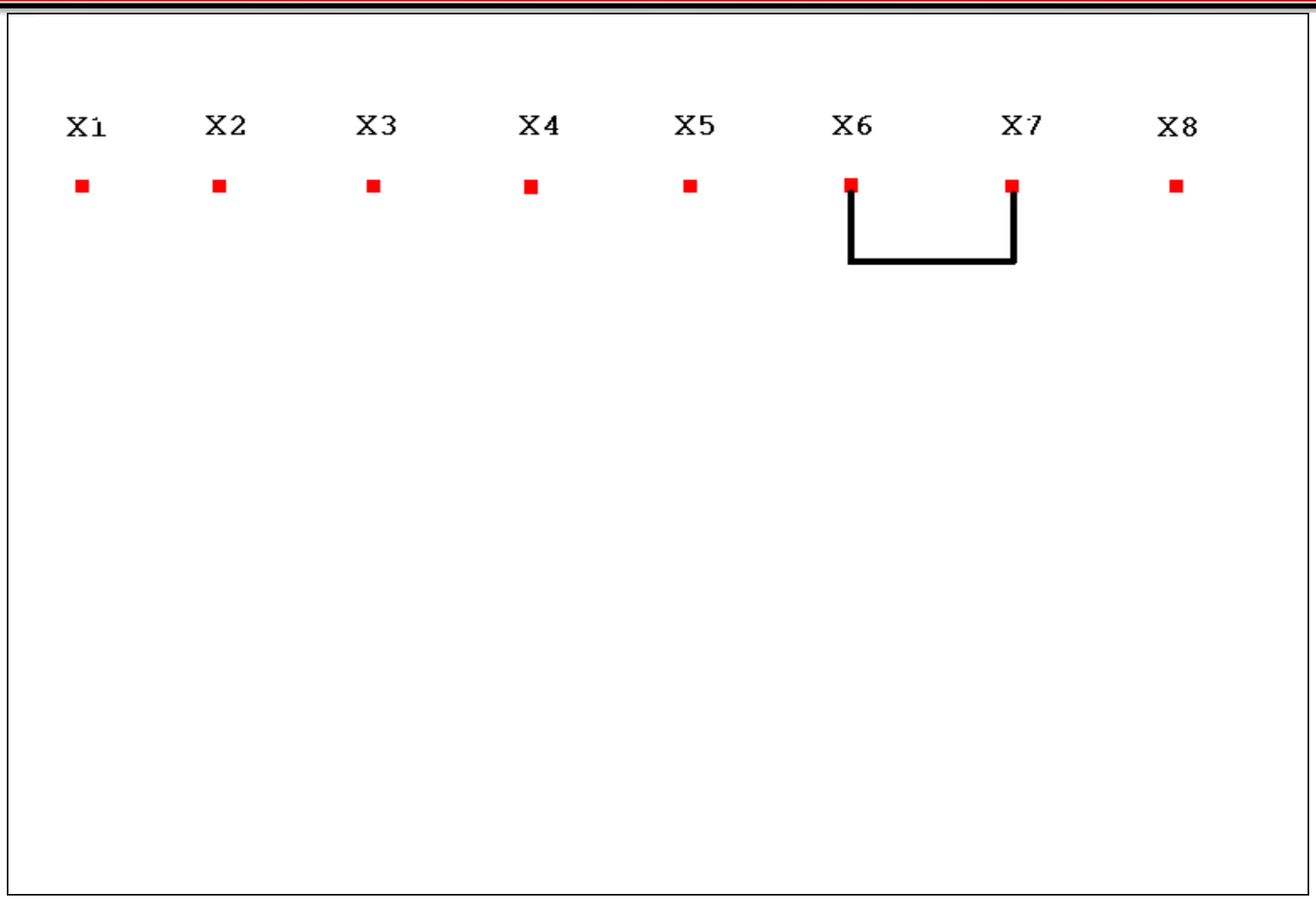
Hierarchical Clustering

- Produces a set of nested clusters organized as a hierarchical tree
- Can be visualized as a "dendrogram"
  - A tree like diagram that records the sequences of merges or splits



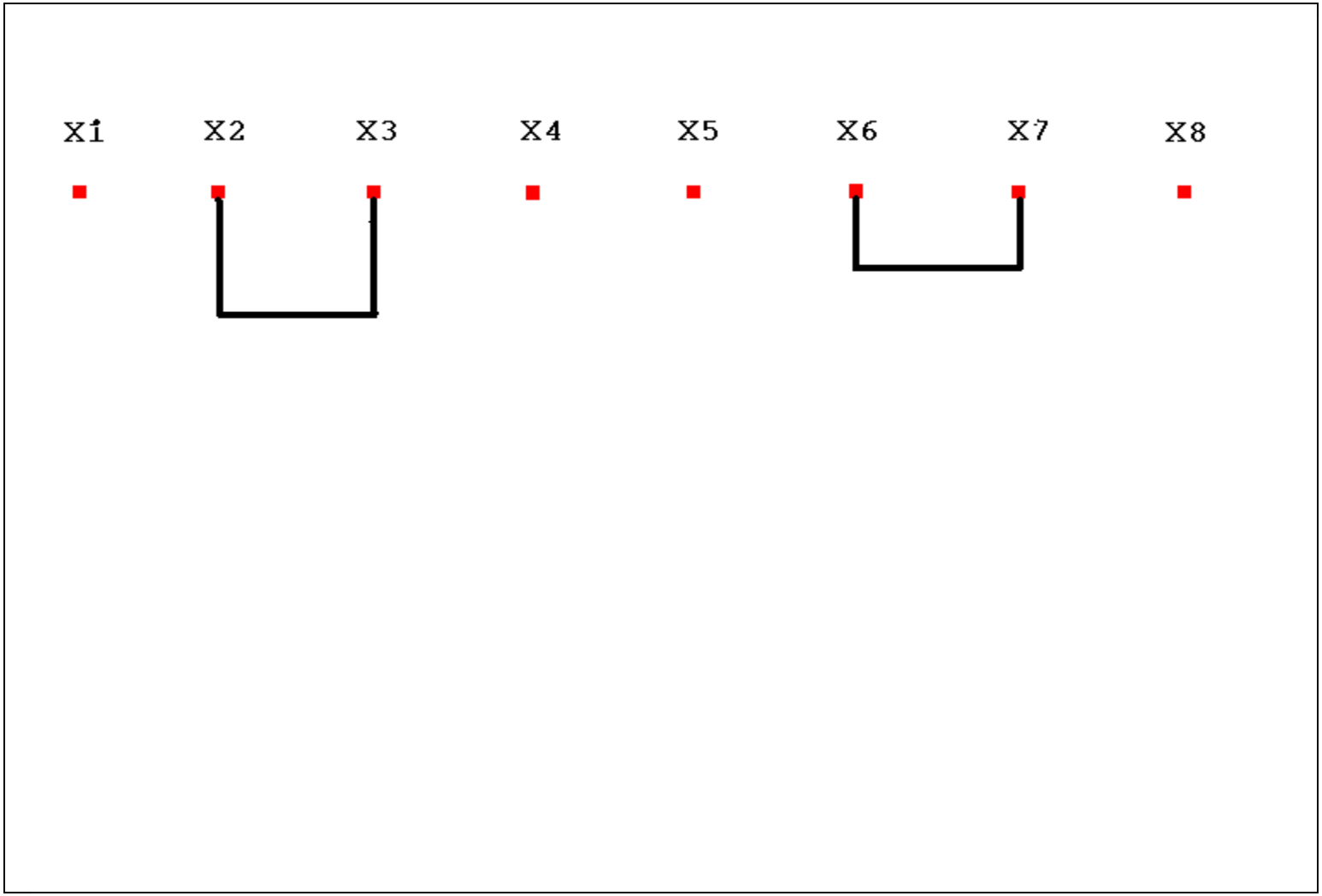


Nearest Neighbor, Level 2, k = 7 clusters.

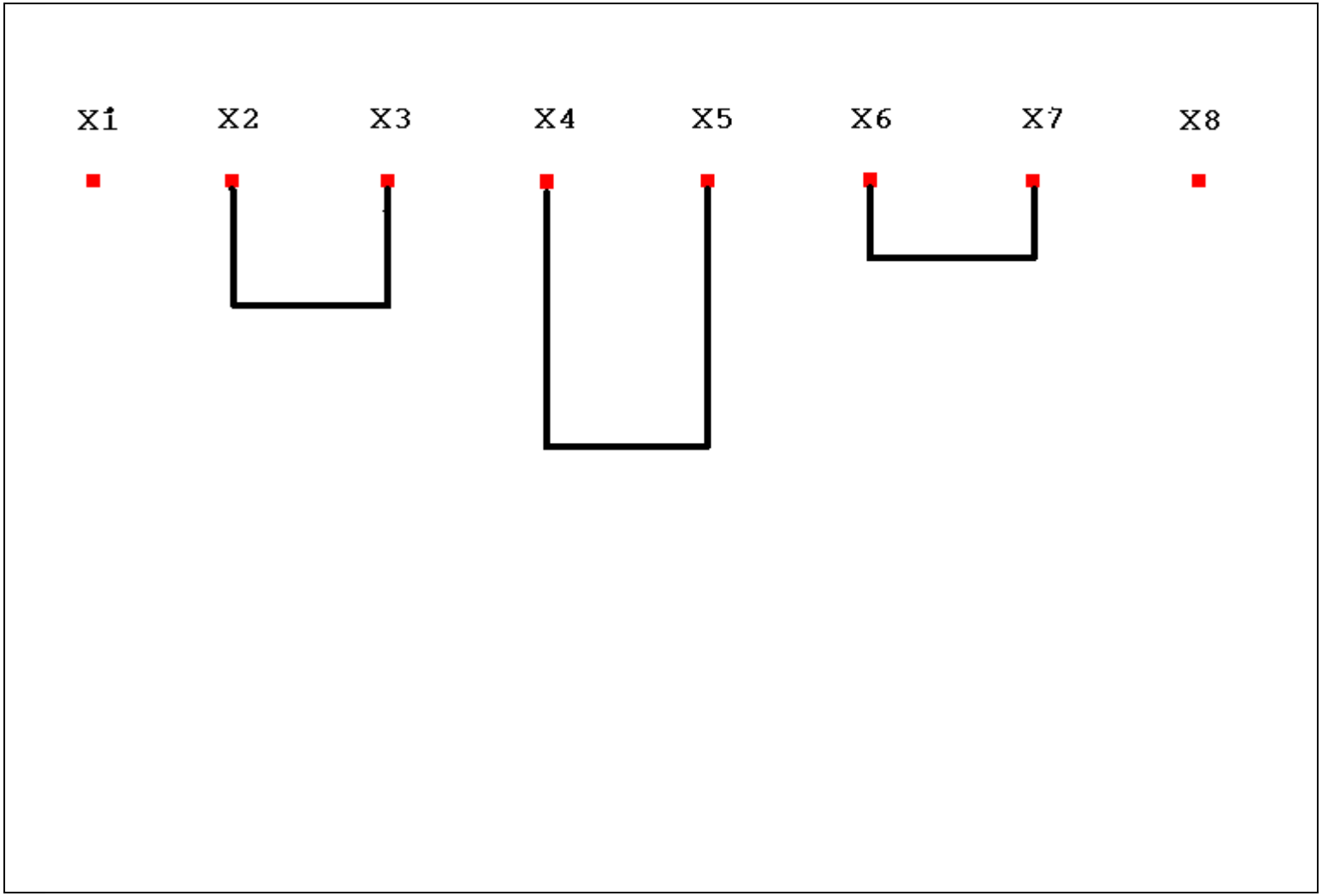


From http://www.stat.unc.edu/postscript/papers/marron/Stat321FDA/RimaIzempresentation.ppt

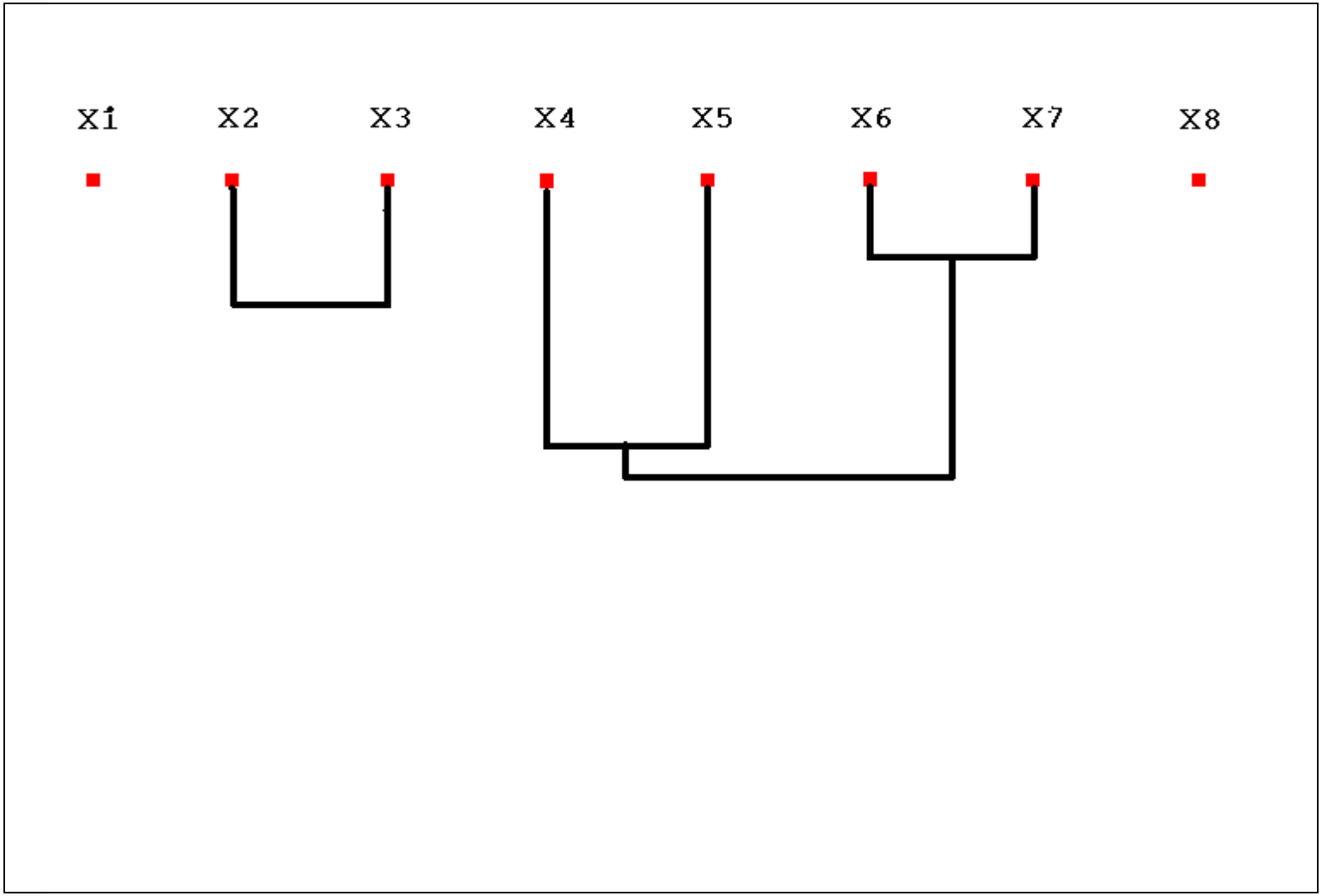
Nearest Neighbor, Level 3, k = 6 clusters.



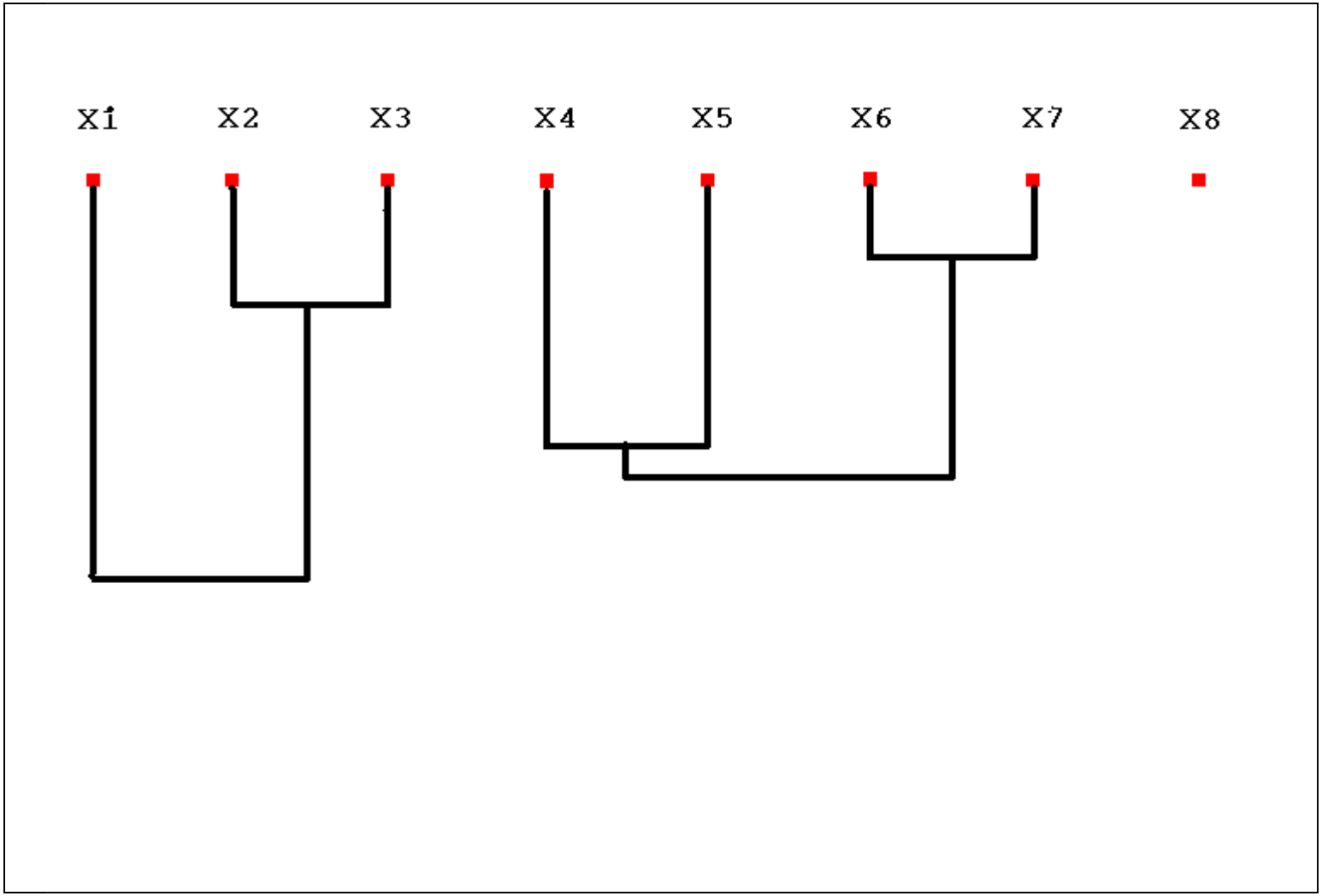
Nearest Neighbor, Level 4, k = 5 clusters.



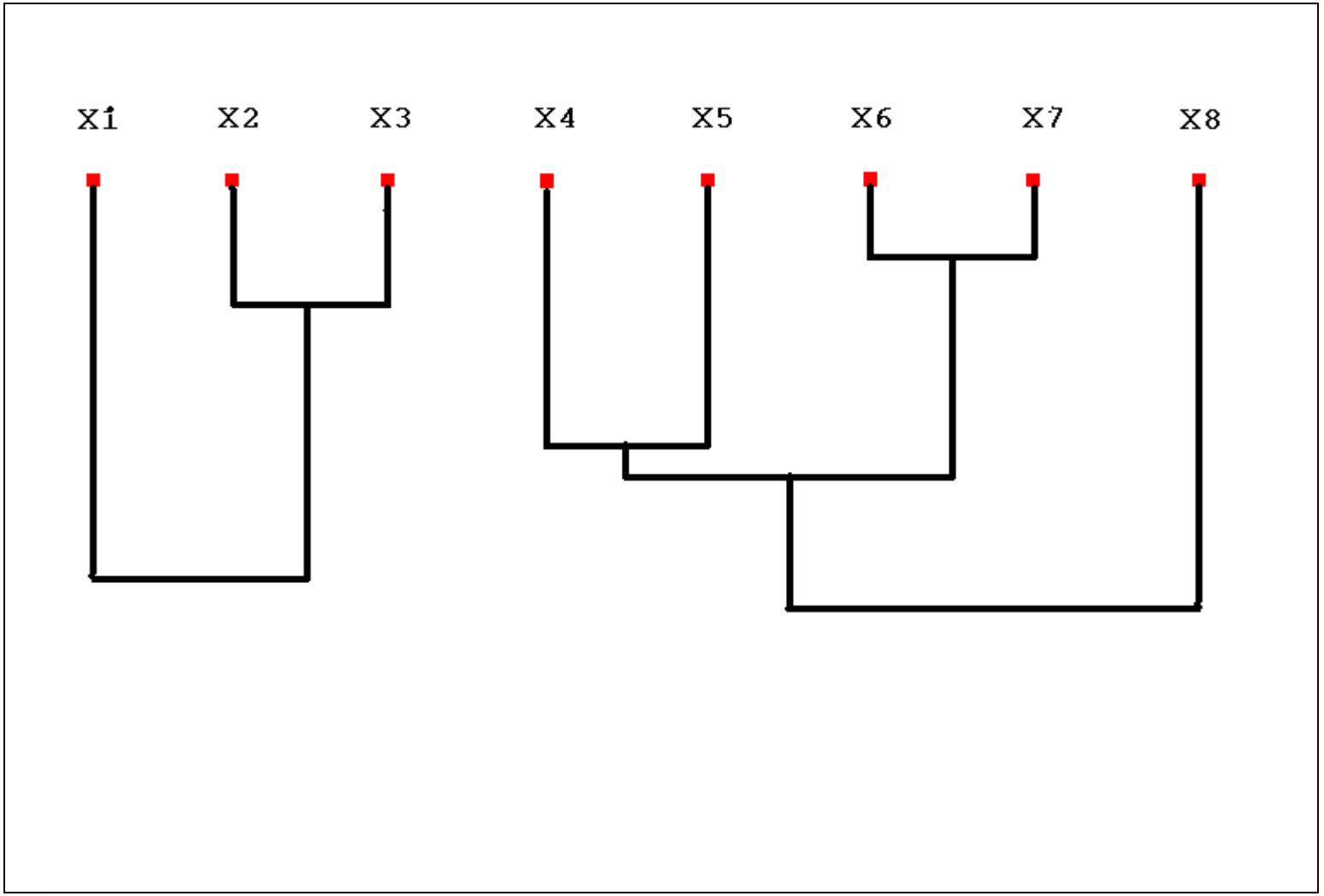
Nearest Neighbor, Level 5, k = 4 clusters.



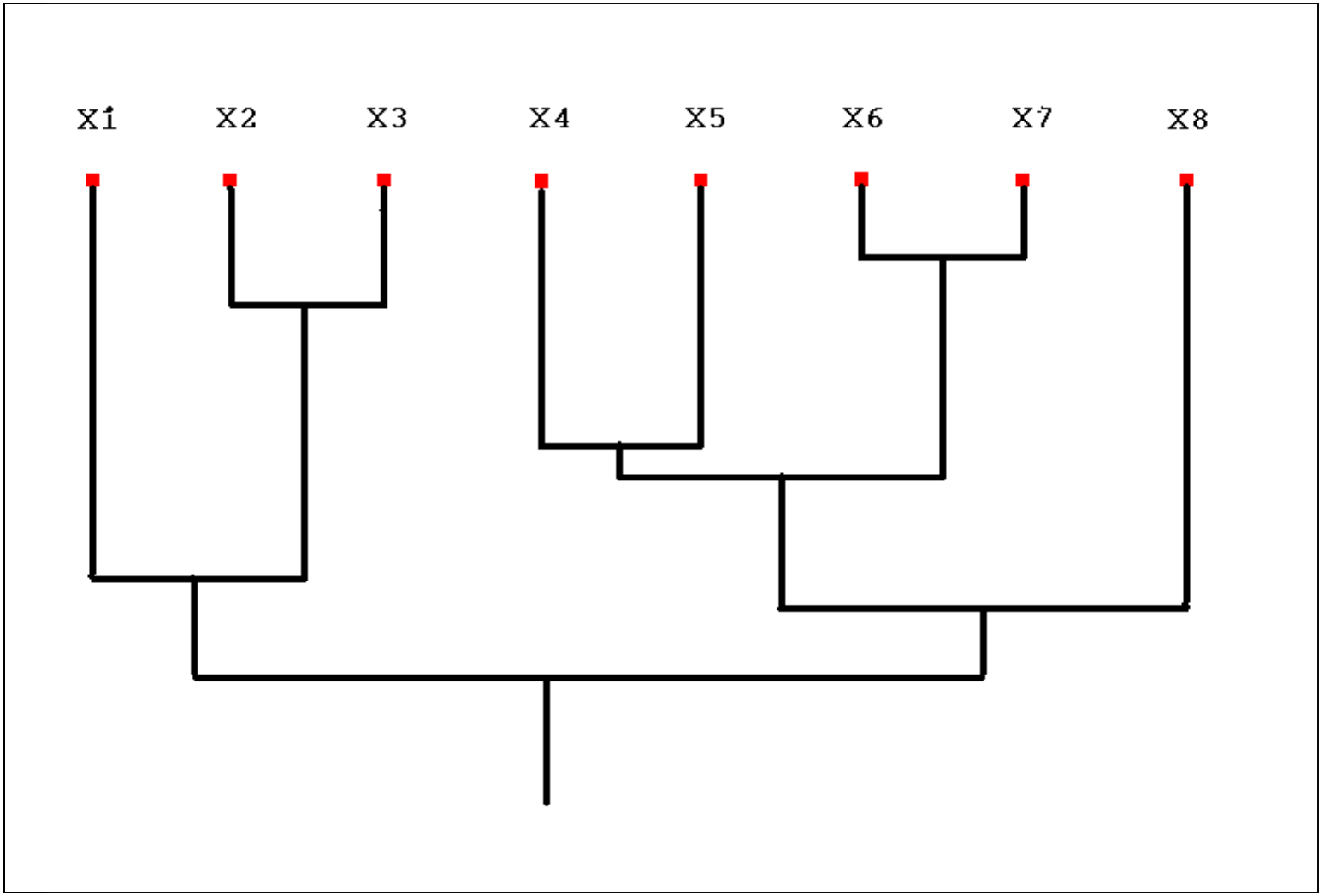
Nearest Neighbor, Level 6, k = 3 clusters.



Nearest Neighbor, Level 7, k = 2 clusters.

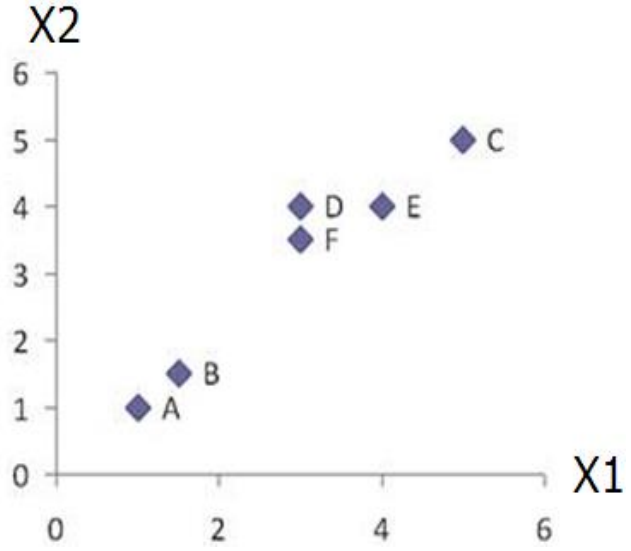


Nearest Neighbor, Level 8, k = 1 cluster.



Example and Demo

- Problem: clustering analysis with agglomerative al



	X1	X2
A	1	1
B	1.5	1.5
C	5	5
D	3	4
E	4	4
F	3	3.5

data matrix

$$d_{AB} = \left((1-1.5)^2 + (1-1.5)^2\right)^{\frac{1}{2}} = \sqrt{\frac{1}{2}} = 0.7071$$

$$d_{DF} = \left((3-3)^2 + (4-3.5)^2\right)^{\frac{1}{2}} = 0.5$$

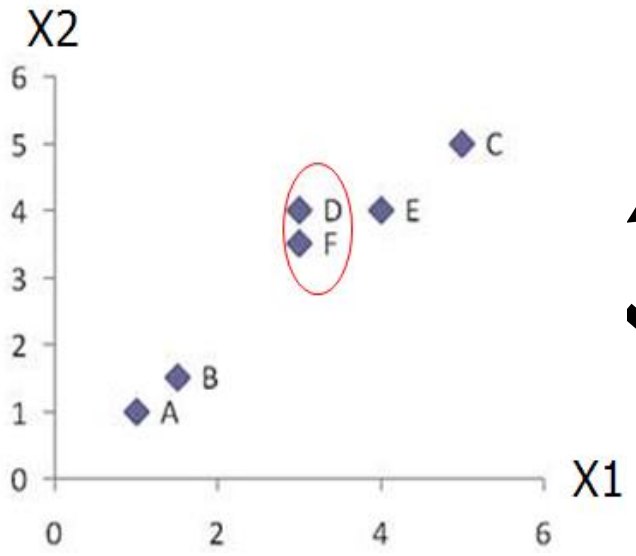
Euclidean distance

Dist	A	B	C	D	E	F
A	0.00	0.71	5.66	3.61	4.24	3.20
B	0.71	0.00	4.95	2.92	3.54	2.50
C	5.66	4.95	0.00	2.24	1.41	2.50
D	3.61	2.92	2.24	0.00	1.00	0.50
E	4.24	3.54	1.41	1.00	0.00	1.12
F	3.20	2.50	2.50	0.50	1.12	0.00

distance matrix

Example and Demo

- Merge two closest clusters



Dist	A	B	C	D	E	F
A	0.00	0.71	5.66	3.61	4.24	3.20
B	0.71	0.00	4.95	2.92	3.54	2.50
C	5.66	4.95	0.00	2.24	1.41	2.50
D	3.61	2.92	2.24	0.00	1.00	0.50
E	4.24	3.54	1.41	1.00	0.00	1.12
F	3.20	2.50	2.50	0.50	1.12	0.00

Dist	A	B	C	D, F	E
A	0.00	0.71	5.66	?	4.24
B	0.71	0.00	4.95	?	3.54
C	5.66	4.95	0.00	?	1.41
D, F	?	?	?	0.00	?
E	4.24	3.54	1.41	?	0.00

Example and Demo

- Update distance matrix

Dist	A	B	C	D	E	F
A	0.00	0.71	5.66	3.61	4.24	3.20
B	0.71	0.00	4.95	2.92	3.54	2.50
C	5.66	4.95	0.00	2.24	1.41	2.50
D	3.61	2.92	2.24	0.00	1.00	0.50
E	4.24	3.54	1.41	1.00	0.00	1.12
F	3.20	2.50	2.50	0.50	1.12	0.00

$$d_{(D,F)\to A} = \min\left(d_{DA}, d_{FA}\right) = \min\left(3.61, 3.20\right) = 3.20$$

$$d_{(D,F)\to B} = \min\left(d_{DB}, d_{FB}\right) = \min\left(2.92, 2.50\right) = 2.50$$

$$d_{(D,F)\to C} = \min\left(d_{DC}, d_{FC}\right) = \min\left(2.24, 2.50\right) = 2.24$$

$$d_{E\to(D,F)} = \min\left(d_{ED}, d_{EF}\right) = \min\left(1.00, 1.12\right) = 1.00$$

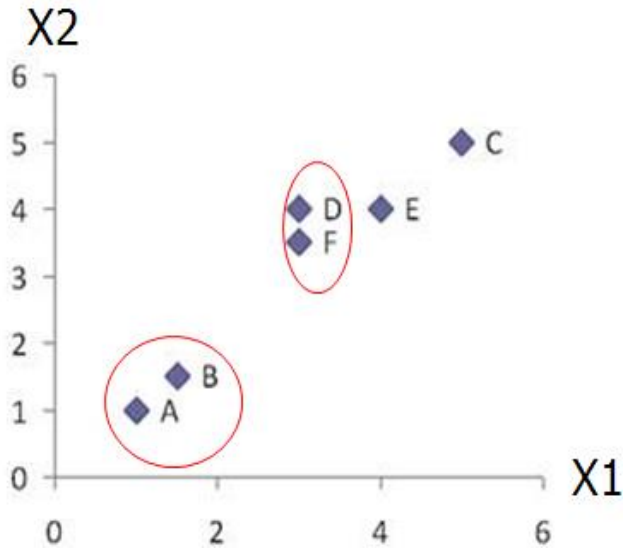
Dist	A	B	C	D, F	E
A	0.00	0.71	5.66	?	4.24
B	0.71	0.00	4.95	?	3.54
C	5.66	4.95	0.00	?	1.41
D, F	?	?	?	0.00	?
E	4.24	3.54	1.41	?	0.00

Min Distance (Single Linkage)

Dist	A	B	C	D, F	E
A	0.00	0.71	5.66	3.20	4.24
B	0.71	0.00	4.95	2.50	3.54
C	5.66	4.95	0.00	2.24	1.41
D, F	**3.20**	**2.50**	**2.24**	0.00	1.00
E	4.24	3.54	1.41	**1.00**	0.00

Example and Demo

- Merge two closest clusters



Min Distance (Single Linkage)

Dist	A	B	C	D, F	E
A	0.00	0.71	5.66	3.20	4.24
B	0.71	0.00	4.95	2.50	3.54
C	5.66	4.95	0.00	2.24	1.41
D, F	**3.20**	**2.50**	**2.24**	0.00	1.00
E	4.24	3.54	1.41	**1.00**	0.00

Dist	A,B	C	(D, F)	E
A,B	0	?	?	?
C	?	0	2.24	1.41
(D, F)	?	2.24	0	1.00
E	?	1.41	1.00	0

Example and Demo

- Update distance matrix

Min Distance (Single Linkage)

Dist	A	B	C	D, F	E
A	0.00	0.71	5.66	3.20	4.24
B	0.71	0.00	4.95	2.50	3.54
C	5.66	4.95	0.00	2.24	1.41
D, F	**3.20**	**2.50**	**2.24**	0.00	1.00
E	4.24	3.54	1.41	**1.00**	0.00

$$d_{C\to(A,B)} = \min\left(d_{CA}, d_{CB}\right) = \min\left(5.66, 4.95\right) = 4.95$$

$$d_{(D,F)\to(A,B)} = \min\left(d_{DA}, d_{DB}, d_{FA}, d_{FB}\right) = \min\left(3.61, 2.92, 3.20, 2.50\right) = 2.50$$

$$d_{E\to(A,B)} = \min\left(d_{EA}, d_{EB}\right) = \min\left(4.24, 3.54\right) = 3.54$$

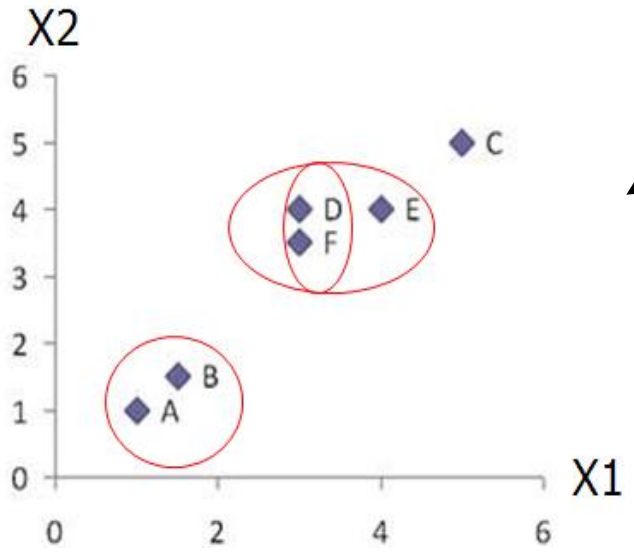
Dist	A,B	C	(D, F)	E
A,B	0	?	?	?
C	?	0	2.24	1.41
(D, F)	?	2.24	0	1.00
E	?	1.41	1.00	0

Min Distance (Single Linkage)

Dist	A,B	C	(D, F)	E
A,B	0	4.95	2.50	3.54
C	**4.95**	0	2.24	1.41
(D, F)	**2.50**	2.24	0	1.00
E	**3.54**	1.41	1.00	0

Example and Demo

- Merge two closest clusters/update distance matrix



Min Distance (Single Linkage)

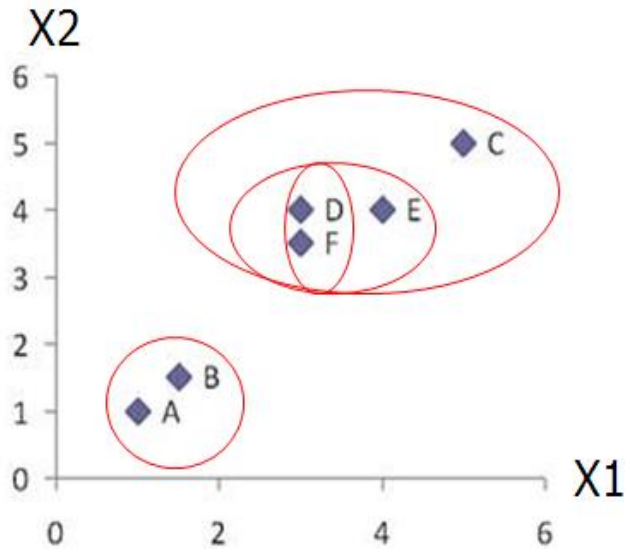
Dist	A,B	C	(D, F)	E
A,B	0	4.95	2.50	3.54
C	**4.95**	0	2.24	1.41
(D, F)	**2.50**	2.24	0	1.00
E	**3.54**	1.41	1.00	0

Min Distance (Single Linkage)

Dist	(A,B)	C	(D, F), E
(A,B)	0.00	4.95	2.50
C	4.95	0.00	1.41
(D, F), E	**2.50**	**1.41**	0.00

Example and Demo

- Merge two closest clusters/update distance matrix



Min Distance (Single Linkage)

Dist	(A,B)	C	(D, F), E
(A,B)	0.00	4.95	2.50
C	4.95	0.00	1.41
(D, F), E	**2.50**	**1.41**	0.00

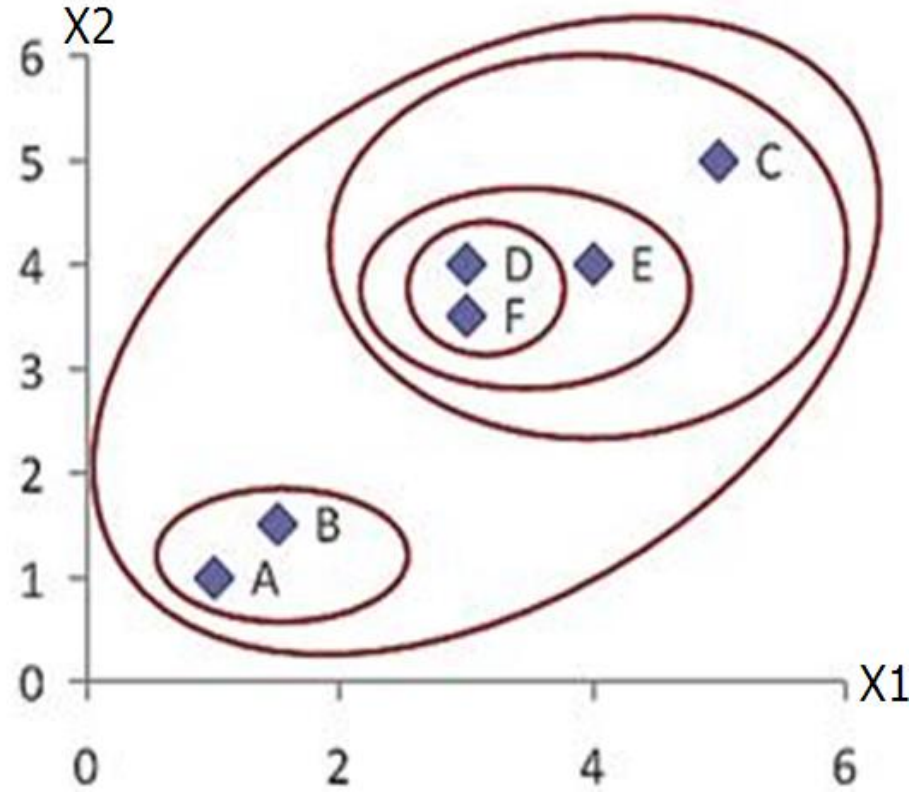
Min Distance (Single Linkage)

Dist	(A,B)	(D, F), E),C
(A,B)	0.00	2.50
((D, F), E),C	**2.50**	0.00

Example and Demo

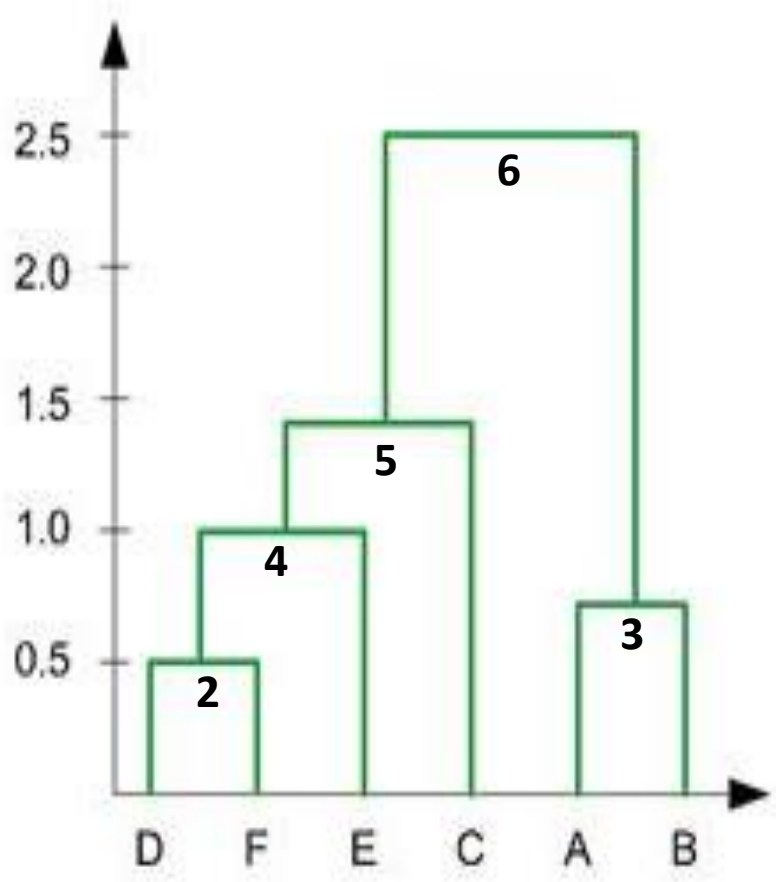
- Final result (meeting termination condition)

	X1	X2
A	1	1
B	1.5	1.5
C	5	5
D	3	4
E	4	4
F	3	3.5



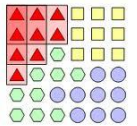
Example and Demo

- Dendrogram tree representation

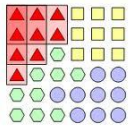


1. In the beginning we have 6 clusters: A, B, C, D, E and F
2. We merge cluster D and F into cluster (D, F) at distance 0.50
3. We merge cluster A and cluster B into (A, B) at distance 0.71
4. We merge cluster E and (D, F) into ((D, F), E) at distance 1.00
5. We merge cluster ((D, F), E) and C into (((D, F), E), C) at distance 1.41
6. We merge cluster (((D, F), E), C) and (A, B) into ((((D, F), E), C), (A, B)) at distance 2.50
7. The last cluster contain all the objects, thus conclude the computation

Density-Based Clustering Methods



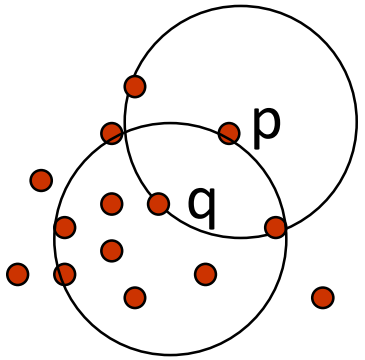
- Clustering based on density (local cluster criterion), such as density-connected points
- Major features:
  - Discover clusters of arbitrary shape
  - Handle noise
  - One scan
  - Need density parameters as termination condition
- Several interesting studies:
  - DBSCAN: Ester, et al. (KDD'96)
  - OPTICS: Ankerst, et al (SIGMOD'99).
  - DENCLUE: Hinneburg & D. Keim (KDD'98)
  - CLIQUE: Agrawal, et al. (SIGMOD'98)



Density-Based Clustering: Background

- Neighborhood of point p=all points within distance Eps from p:
  - $N_{Eps}(p)=\{q \mid dist(p,q) <= Eps\}$
- Two parameters***:***
  - ***Eps***: Maximum radius of the neighbourhood
  - ***MinPts***: Minimum number of points in an Eps-neighbourhood of that point
- If the number of points in the Eps-neighborhood of p is at least ***MinPts***, then p is called a core object.
- Directly density-reachable**:** A point ***p*** is directly density-reachable from a point ***q*** wrt. ***Eps***, ***MinPts*** if
  - 1) ***p*** belongs to $\boldsymbol{N_{Eps}(q)}$
  - 2) core point condition:

$$|\boldsymbol{N_{Eps}(q)}| >= \boldsymbol{MinPts}$$

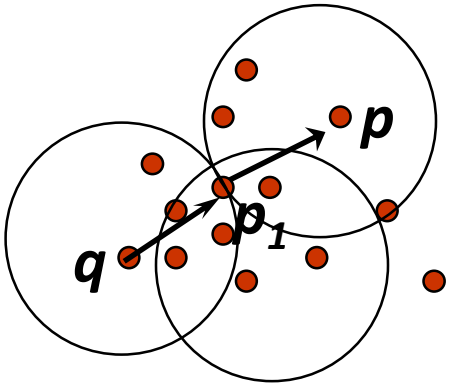


MinPts = 5

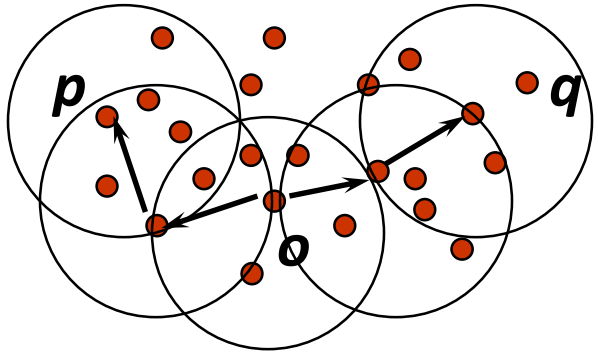
Eps = 1 cm

Density-Based Clustering: Background (II)

- Density-reachable:
  - A point *p* is density-reachable from a point *q* wrt. *Eps*, *MinPts* if there is a chain of points $p_1, \ldots, p_n, p_1 = q, p_n = p$ such that p_{i+1} is directly density-reachable from p_i

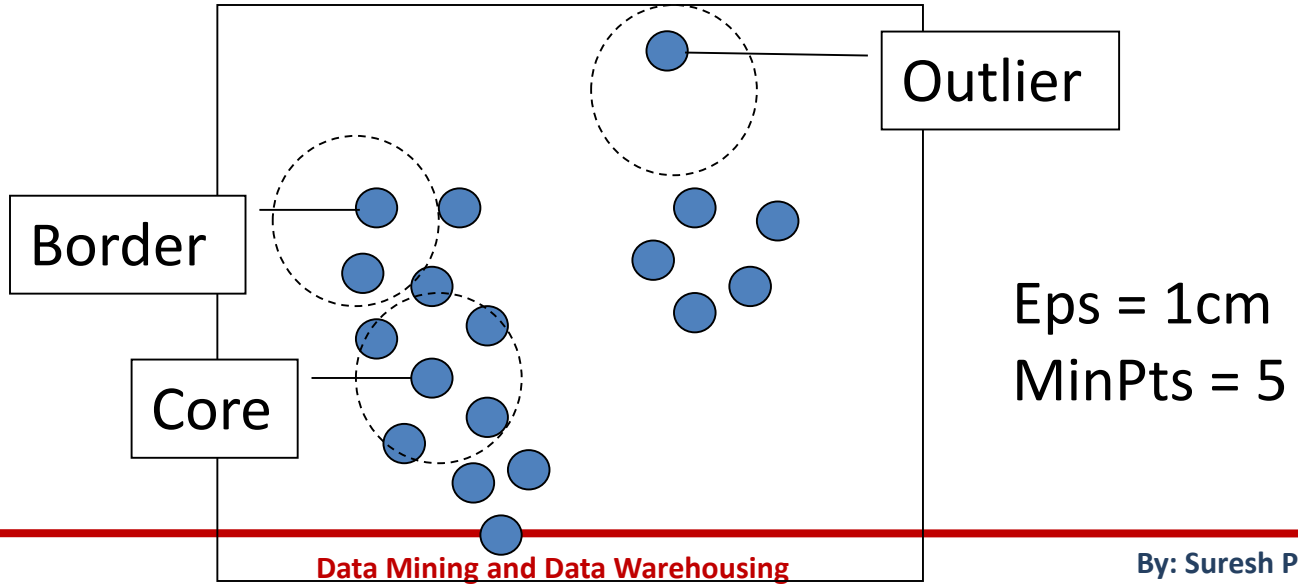


- Density-connected
  - A point *p* is density-connected to a point *q* wrt. *Eps*, *MinPts* if there is a point *o* such that both, *p* and *q* are density-reachable from *o* wrt. *Eps* and *MinPts*.

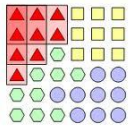


DBSCAN: Density Based Spatial Clustering of Applications with Noise

- Relies on a *density-based* notion of cluster: A *cluster* is defined as a maximal set of density-connected points
- Discovers clusters of arbitrary shape in spatial databases with noise



DBSCAN: The Algorithm



- Arbitrary select a point ***p***
- Retrieve all points density-reachable from ***p*** wrt ***Eps*** and ***MinPts***.
- If ***p*** is a core point, a cluster is formed.
- If ***p*** is a border point, no points are density-reachable from ***p*** and DBSCAN visits the next point of the database.
- Continue the process until all of the points have been processed.