بسم الله الرحمن الرحیم

بازشناسی الگو

درس ۱۴

خوشه‌بندی: مفاهیم پایه

Clustering: Basic Concepts

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مقدمه

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خوشه‌بندی

PATTERN RECOGNITION

بازشناسی الگو
Pattern Recognition

نسبت‌دهی الگوها به طبقه‌های متناظر با آنها

طبقه‌بندی
Classification

بازشناسی با هدف دسته‌بندی الگوها
در طبقه‌های از پیش معلوم

طبقه
Class

خوشه‌بندی
Clustering

بازشناسی با هدف دسته‌بندی الگوها
در **خوشه‌های از پیش نامعلوم** (اما معیار شباهت معلوم)

خوشه
Cluster

CLUSTERING

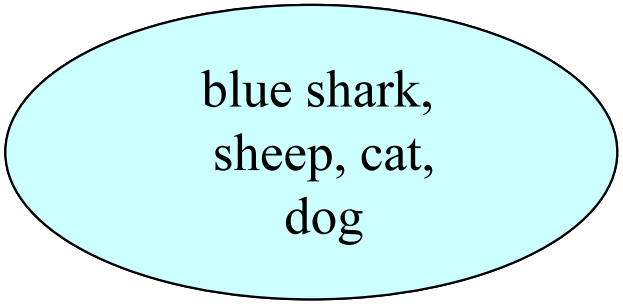
❖ Basic Concepts

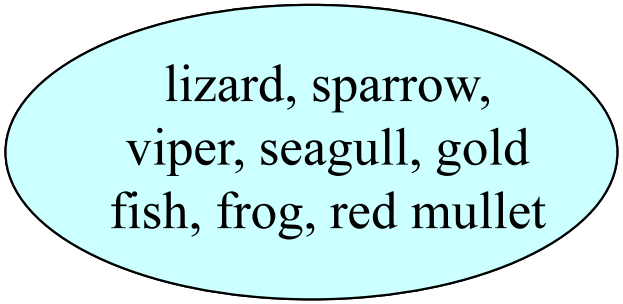
In clustering or unsupervised learning no training data, with class labeling, are available. The goal becomes: Group the data into a number of sensible clusters (groups). This unravels similarities and differences among the available data.

- **Applications:**
  - Engineering
  - Bioinformatics
  - Social Sciences
  - Medicine
  - Data Mining and Web Mining

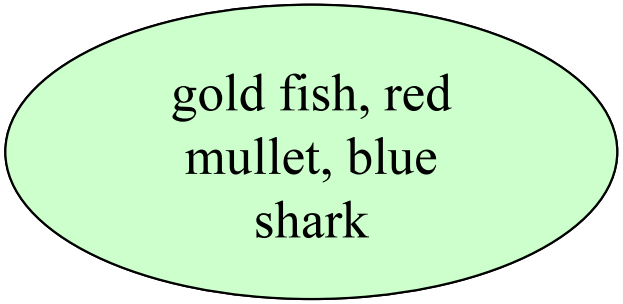
- To perform clustering of a data set, a clustering criterion must first be adopted. Different clustering criteria lead, in general, to different clusters.

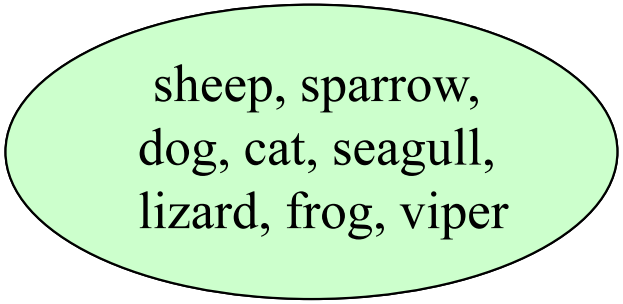
➢ A simple example





1. Two clusters
2. **Clustering criterion:**
   How animals bear their progeny



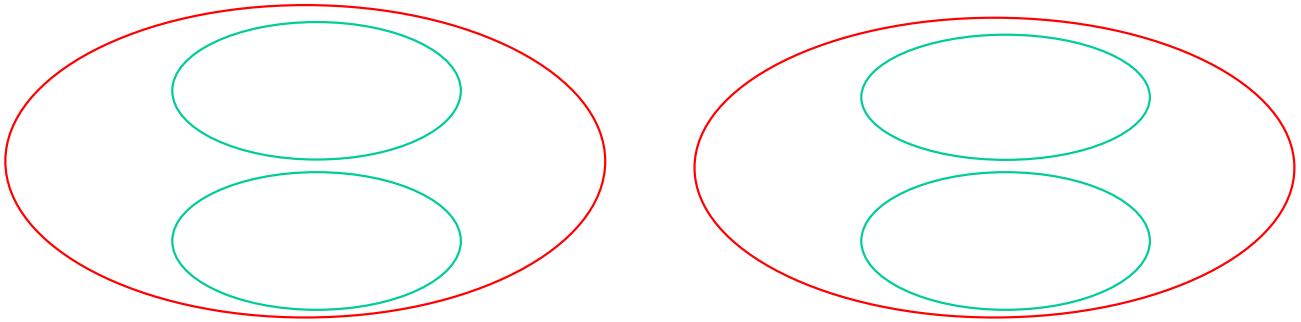


1. Two clusters
2. **Clustering criterion:**
   Existence of lungs

❖ 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.

- 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.
- A simple example: How many clusters??



2 or 4 ??

❖ Basic application areas for clustering

- **Data reduction.**
  All data vectors within a cluster are substituted (represented) by the corresponding cluster representative.
- **Hypothesis generation.**
- **Hypothesis testing.**
- **Prediction based on groups.**

❖ Clustering Definitions

➢ **Hard Clustering:** Each point belongs to a single cluster

- Let $X = \{\underline{x}_1, \underline{x}_2, \ldots, \underline{x}_N\}$

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

$$C_i \neq \emptyset, \; i = 1,2,\ldots,m$$

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

$$C_i \bigcap C_j = \emptyset, \;\; i \neq j, \;\; i, j = 1,2,\ldots, m$$

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

Quantifying the terms similar-dissimilar depends on the types of clusters that are expected to underlie the structure of X.

- **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

$$u_j : X \to [0,1], \quad j = 1,2,\ldots,m$$

$$\sum_{j=1}^{m} u_j(\underline{x}_i) = 1, \quad i = 1,2,\ldots,N$$

$$0 < \sum_{i=1}^{N} u_j(\underline{x}_i) < N, \quad j = 1,2,\ldots,m$$

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

$$u_j(\underline{x}_i), \quad j = 1,2,\ldots,m$$

$u_j(\underline{x}_i)$ 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.

TYPES OF FEATURES

- With respect to their domain
  - 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 sex 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).

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معیارهای نزدیکی

معیارهای نزدیکی

PROXIMITY MEASURES

معیار نزدیکی
Proximity Measure

معیار عدم شباهت (فاصله)
Dissimilarity Measure (Distance)

معیار شباهت
Similarity Measure

بین بردارها
Between Vectors

بین مجموعه‌ها
Between Sets

بین بردار و مجموعه
Between a Vector and a Set

PROXIMITY MEASURES

❖ *Between vectors*

➢ Dissimilarity measure (between vectors of X) is a function

$$d: \; X \times X \longrightarrow R$$

with the following properties

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

If in addition

- $d(\underline{x}, \underline{y}) = d_0 \ \textit{if and only if} \ \underline{x} = \underline{y}$
- $d(\underline{x}, \underline{z}) \leq d(\underline{x}, \underline{y}) + d(\underline{y}, \underline{z}), \ \forall \underline{x}, \underline{y}, \underline{z} \in X$

  (triangular inequality)

d is called a metric dissimilarity measure.

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

$$s: \; X \times X \longrightarrow R$$

with the following properties

- $\exists s_0 \in R: \; -\infty < s(\underline{x}, \underline{y}) \leq s_0 < +\infty, \;\; \forall \underline{x}, \underline{y} \in X$
- $s(\underline{x}, \underline{x}) = s_0, \;\; \forall \underline{x} \in X$
- $s(\underline{x}, \underline{y}) = s(\underline{y}, \underline{x}), \;\; \forall \underline{x}, \underline{y} \in X$

If in addition

- $s(\underline{x}, \underline{y}) = s_0 \ \textit{if and only if} \ \underline{x} = \underline{y}$
- $s(\underline{x}, \underline{y})s(\underline{y}, \underline{z}) \leq [s(\underline{x}, \underline{y}) + s(\underline{y}, \underline{z})]s(\underline{x}, \underline{z}), \quad \forall \underline{x}, \underline{y}, \underline{z} \in X$

s is called a metric similarity measure.

❖ *Between sets*

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

A proximity measure $\wp$ on U is a function

$$\wp : U \times U \longrightarrow R$$

A dissimilarity measure has to satisfy the relations of dissimilarity measure between vectors, where D_i's are used in place of $\underline{x}$, $\underline{y}$ (similarly for similarity measures).

PROXIMITY MEASURES BETWEEN VECTORS

❖ Real-valued vectors

➢ **Dissimilarity measures** (DMs)

• *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)

– $p = \infty$ ($d_\infty(\underline{x},\underline{y}) = \max_{1 \le i \le l} w_i \mid x_i - y_i \mid$)

- *Other measures*
  - $$d_G(\underline{x},\underline{y}) = -\log_{10}\left(1-\frac{1}{l}\sum_{j=1}^{l}\frac{|x_j - y_j|}{b_j - a_j}\right)$$

    where b_j and a_j are the maximum and the minimum values of the j-th feature, among the vectors of X (dependence on the current data set)

  - $$d_Q(\underline{x},\underline{y}) = \sqrt{\frac{1}{l}\sum_{j=1}^{l}\left(\frac{x_j - y_j}{x_j + y_j}\right)^2}$$

➢ 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*

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

- $$s_T(\underline{x}, \underline{y}) = 1 - \frac{d_2(\underline{x}, \underline{y})}{\| \underline{x} \| + \| \underline{y} \|}$$

❖ Discrete-valued vectors

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

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)

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

  - The l_1 distance

$$d_1(\underline{x},\underline{y}) = \sum_{i=1}^{l} |\, x_i - y_i \,|$$

➢ Similarity measures:

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

- Measures that exclude a_{00}: $$\sum_{i=1}^{k-1} a_{ii} / l \qquad \sum_{i=1}^{k-1} a_{ii} /(l - a_{00})$$

- Measures that include a_{00}: $$\sum_{i=0}^{k-1} a_{ii} / l$$

❖ Mixed-valued vectors

Some of the coordinates of the vectors $\underline{\boldsymbol{x}}$ are real and the rest are discrete.

Methods for measuring the proximity between two such $\underline{x}_i$ and $\underline{x}_j$:

- Adopt a proximity measure (PM) suitable for real-valued vectors.
- Convert the real-valued features to discrete ones and employ a discrete PM.

The more general case of mixed-valued vectors:

- Here nominal, ordinal, interval-scaled, ratio-scaled features are treated separately.

The similarity function between $\underline{x}_i$ and $\underline{x}_j$ is:

$$s(\underline{x}_i, \underline{x}_j) = \sum_{q=1}^{l} s_q(\underline{x}_i, \underline{x}_j) / \sum_{q=1}^{l} w_q$$

In the above definition:

- $w_q = 0$, if at least one of the q-th coordinates of $\underline{x}_i$ and $\underline{x}_j$ *are* undefined or both the q-th coordinates are equal to 0. Otherwise $w_q = 1$.
- If the q-th coordinates are binary, $s_q(\underline{x}_i,\underline{x}_j) = 1$ if $x_{iq}=x_{jq}=1$ and 0 otherwise.
- If the q-th coordinates are nominal or ordinal, $s_q(x_i,xj) = 1$ if $x_{iq}=x_{jq}$ and 0 otherwise.
- If the q-th coordinates are interval or ratio scaled-valued

$$s_q(\underline{x}_i, \underline{x}_j) = 1 - |\, x_{iq} - x_{jq} \,| / r_q,$$

where r_q is the interval where the q-th coordinates of the vectors of the data set X lie.

❖ Fuzzy measures

Let $\underline{x}, \underline{y} \in [0,1]^l$. Here the value of the i-th coordinate, x_i, of $\underline{x}$, is **not** the outcome of a measuring device.

- The closer the coordinate x_i is to 1 (0), the more likely the vector $\underline{x}$ possesses (does not possess) the i-th characteristic.
- As x_i approaches 0.5, the certainty about the possession or not of the i-th feature from $\underline{x}$ decreases.

$$s(x_i, y_i) = \max(\min(1 - x_i, 1 - y_i), \min(x_i, y_i))$$

A possible similarity measure that can quantify the above is:

Then $$s_F^q(\underline{x}, \underline{y}) = \left(\sum_{i=1}^{l} s(x_i, y_i)^q \right)^{1/q}$$

❖ Missing data

For some vectors of the data set X, some features values are unknown

Ways to face the problem:

- Discard all vectors with missing values (not recommended for small data sets)
- Find the mean value m_i of the available i-th feature values over that data set and substitute the missing i-th feature values with m_i.
- Define $b_i = 0$, if both the i-*th* features x_i, y_i are available and 1 otherwise. Then

$$\wp(\underline{x}, \underline{y}) = \frac{l}{l - \sum_{i=1}^{l} b_i} \sum_{all\ i:\ b_i=0} \phi(x_i, y_i)$$

where $\phi(x_i, y_i)$ denotes the PM between two scalars x_i, y_i.

- Find the average proximities $\phi_{avg}(i)$ between all feature vectors in X along all components. Then

$$\wp(\underline{x}, \underline{y}) = \sum_{i=1}^{l} \psi(x_i, y_i)$$

where $\psi(x_i, y_i) = \phi(x_i, y_i)$, if both x_i and y_i are available and $\phi_{avg}(i)$ otherwise.

PROXIMITY FUNCTIONS BETWEEN A VECTOR AND A SET

❖ Let $X = \{\underline{x}_1, \underline{x}_2, \ldots, \underline{x}_N\}$ and $C \subset X$, $\underline{x} \in X$

❖ *All points of C contribute to the definition of* $\wp(\underline{x}, C)$

➢ Max proximity function

$$\wp^{ps}_{\max}(\underline{x}, C) = \max_{\underline{y} \in C} \wp(\underline{x}, \underline{y})$$

➢ Min proximity function

$$\wp^{ps}_{\min}(\underline{x}, C) = \min_{\underline{y} \in C} \wp(\underline{x}, \underline{y})$$

➢ Average proximity function

$$\wp^{ps}_{avg}(\underline{x}, C) = \frac{1}{n_C} \sum_{\underline{y} \in C} \wp(\underline{x}, \underline{y})$$

n_C is the cardinality of C

❖ *A representative(s) of C, r_C, contributes to the definition of $\wp(x,C)$*

In this case: $\wp(x,C)=\wp(x,r_C)$

Typical representatives are:

➢ The mean vector:

$$\underline{m}_p = \left(1/n_C\right)\sum_{y\in C}\underline{y}$$

where n_C is the cardinality of C

➢ The mean center:

$$\underline{m}_C \in C: \sum_{\underline{y}\in C} d(\underline{m}_C,\underline{y}) \le \sum_{\underline{y}\in C} d(\underline{z},\underline{y}),\ \forall \underline{z}\in C$$

d: a dissimilarity measure

➢ The median center:

$$\underline{m}_{med} \in C: \text{ med}(d(\underline{m}_{med},\underline{y}) \mid \underline{y}\in C) \le \text{med}(d(\underline{z},\underline{y}) \mid \underline{y}\in C),\ \forall \underline{z}\in C$$

NOTE: Other representatives (e.g., hyperplanes, hyperspheres) are useful in certain applications (e.g., object identification using clustering techniques).

PROXIMITY FUNCTIONS BETWEEN SETS

- Let $X = \{\underline{x}_1, \ldots, \underline{x}_N\}$, D_i, $D_j \subset X$ and $n_i = |D_i|$, $n_j = |D_j|$
- All points of each set contribute to $\wp(D_i, D_j)$
  - Max proximity function (measure but not metric, only if $\wp$ is a similarity measure)

$$\wp^{ss}_{\max}(D_i, D_j) = \max_{\underline{x} \in D_i, \underline{y} \in D_j} \wp(\underline{x}, \underline{y})$$

  - Min proximity function (measure but not metric, only if $\wp$ is a dissimilarity measure)

$$\wp^{ss}_{\min}(D_i, D_j) = \min_{\underline{x} \in D_i, \underline{y} \in D_j} \wp(\underline{x}, \underline{y})$$

  - Average proximity function (not a measure, even if $\wp$ is a measure)

$$\wp^{ss}_{avg}(D_i, D_j) = \left(1 / n_i n_j \right) \sum_{x \in D_i} \sum_{x \in D_j} \wp(\underline{x}, \underline{y})$$

❖ Each set D_i is represented by its representative vector $\underline{m}_i$

➢ Mean proximity function
(it is a measure provided that $\wp$ is a measure):

$$\wp^{ss}_{mean}(D_i, D_j) = \wp(\underline{m}_i, \underline{m}_j)$$

➢ $$\wp^{ss}_{e}(D_i, D_j) = \sqrt{\frac{n_i n_j}{n_i + n_j}}\wp(\underline{m}_i, \underline{m}_j)$$

NOTE: Proximity functions between a vector $\underline{x}$ and a set C may be derived from the above functions if we set $D_i = \{\underline{x}\}$.

➢ Remarks:

- Different choices of proximity functions between sets may lead to totally different clustering results.

- Different proximity measures between vectors in the same proximity function between sets may lead to totally different clustering results.

- The only way to achieve a proper clustering is
  - by trial and error and,
  - taking into account the opinion of an expert in the field of application.

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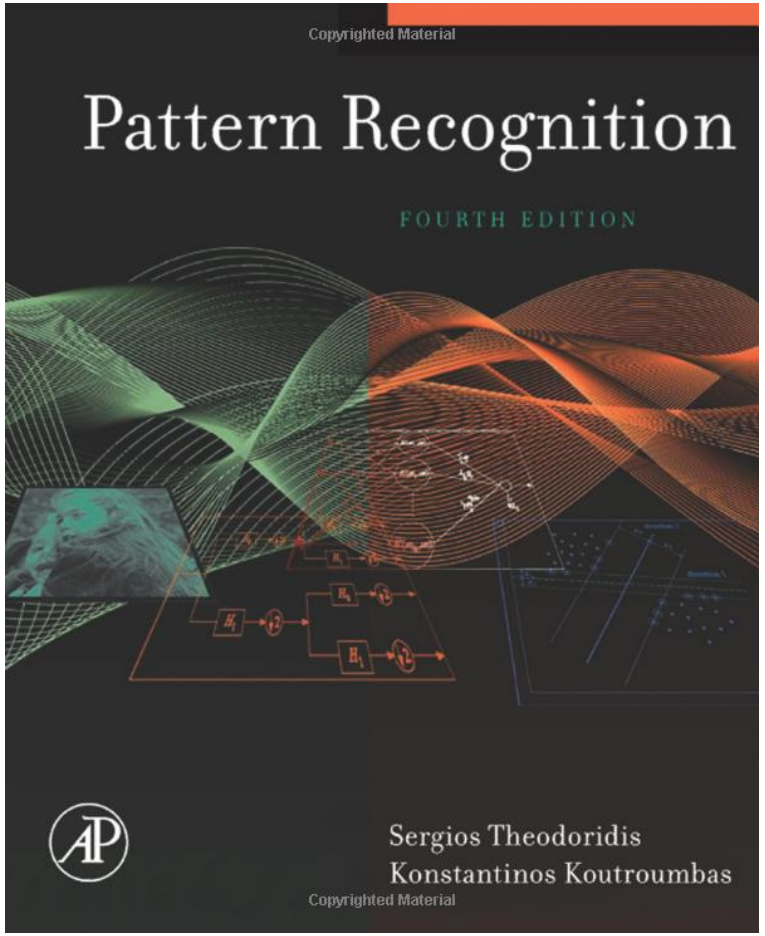
منابع

منبع اصلی



S. Theodoridis, K. Koutroumbas,
Pattern Recognition,
Fourth Edition, Academic Press, 2009.

Chapter 11

CHAPTER

Clustering: Basic Concepts 11

11.1 INTRODUCTION

All the previous chapters were concerned with supervised classification. In the current and following chapters, we turn to the unsupervised case, where class labeling of the training patterns is not available. Thus, our major concern now is to "reveal" the organization of patterns into "*sensible*" clusters (groups), which will allow us to discover similarities and differences among patterns and to derive useful conclusions about them. This idea is met in many fields, such as the life sciences (biology, zoology), medical sciences (psychiatry, pathology), social sciences (sociology, archaeology), earth sciences (geography, geology), and engineering [Ande 73]. Clustering may be found under different names in different contexts, such as unsupervised learning and learning without a teacher (in pattern recognition), numerical taxonomy (in biology, ecology), typology (in social sciences), and partition (in graph theory). The following example is inspired by biology and gives us a flavor of the problem.

Consider the following animals: sheep, dog, cat (mammals), sparrow, seagull (birds), viper, lizard (reptiles), goldfish, red mullet, blue shark (fish), and frog (amphibians). In order to organize these animals into clusters, we need to define a *clustering criterion*. Thus, if we employ the way these animals bear their progeny as a clustering criterion, the sheep, the dog, the cat, and the blue shark will be assigned to the same cluster, while all the rest will form a second cluster (Figure 11.1a). If the clustering criterion is the existence of lungs, the goldfish, the red mullet, and the blue shark are assigned to the same cluster, while all the other animals are assigned to a second cluster (Figure 11.1b). On the other hand, if the clustering criterion is the environment where the animals live, the sheep, the dog, the cat, the sparrow, the seagull, the viper, and the lizard will form one cluster (animals living outside water); the goldfish, the red mullet, and the blue shark will form a second cluster (animals living only in water); and the frog will form a third cluster by itself, since it may live in the water or out of it (Figure 11.1c). It is worth pointing out that if the existence of a vertebral column is the clustering criterion, all the animals will lie in the same cluster. Finally, we may use composite clustering criteria as

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