Chapter 5: Clustering

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致谢:课件主要参考《 Mining of Massive Datasets》(Second Edition) J. Leskovec, A. Rajaraman, J. Ullman的相关课件, 特此致谢!!!

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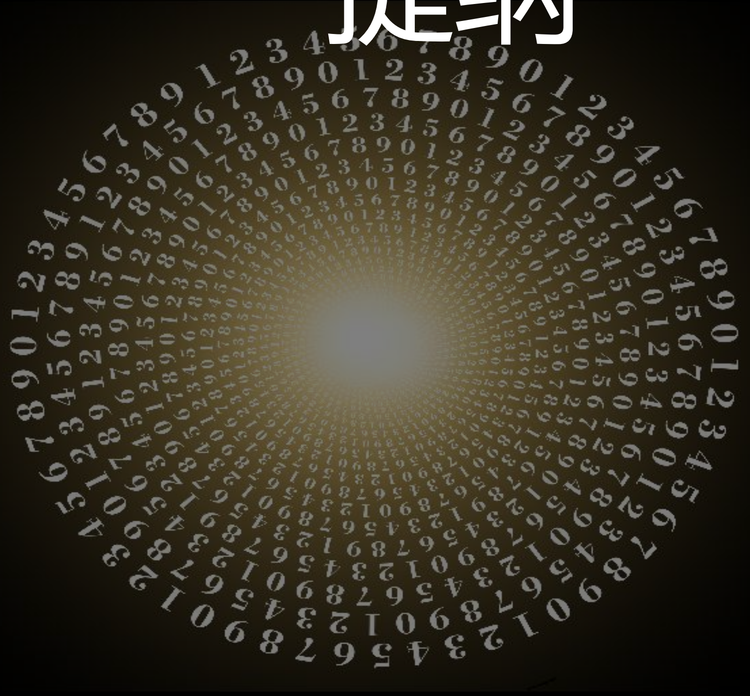
提纲



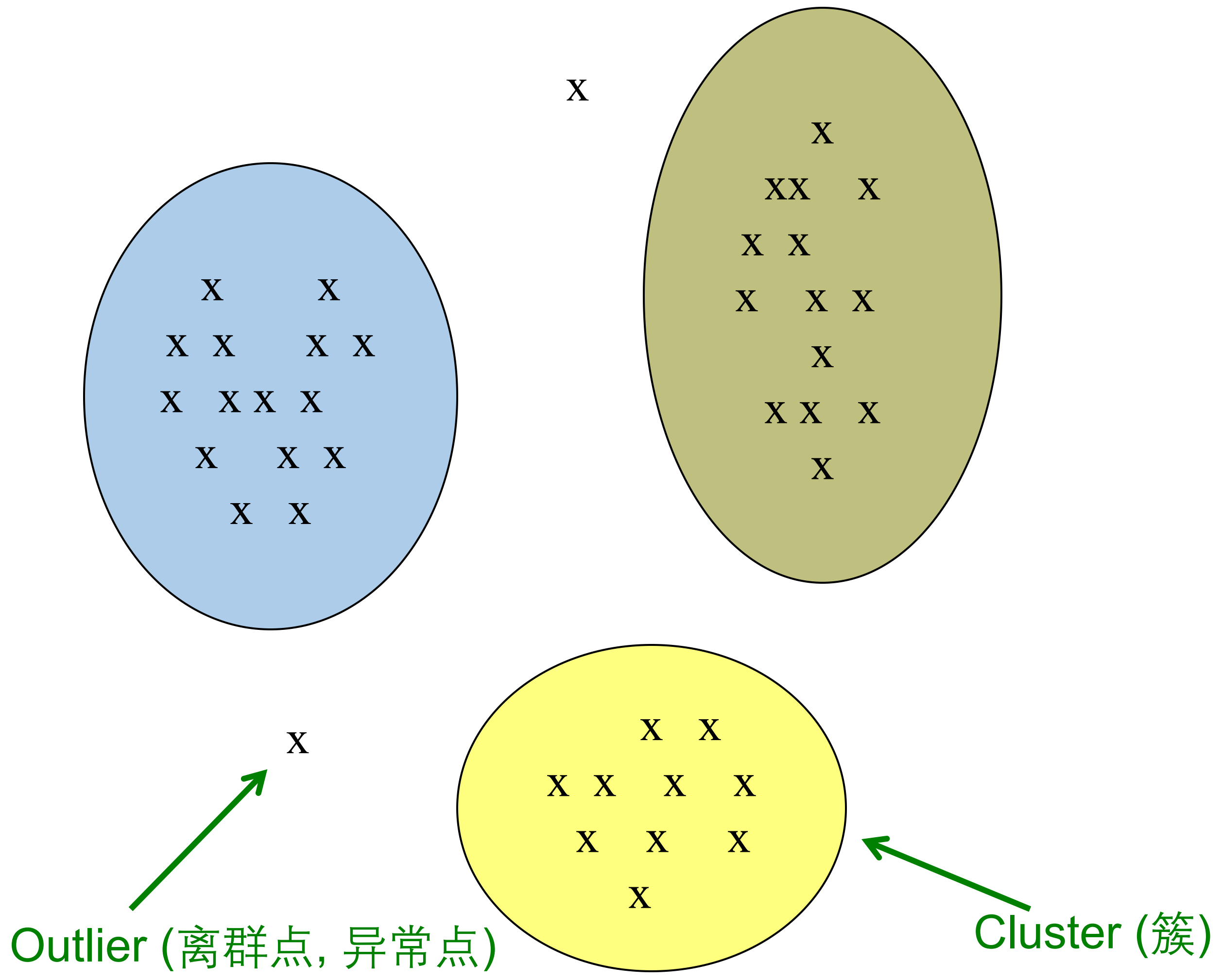
High Dimensional Data

- Given a cloud of data points we want to understand its structure

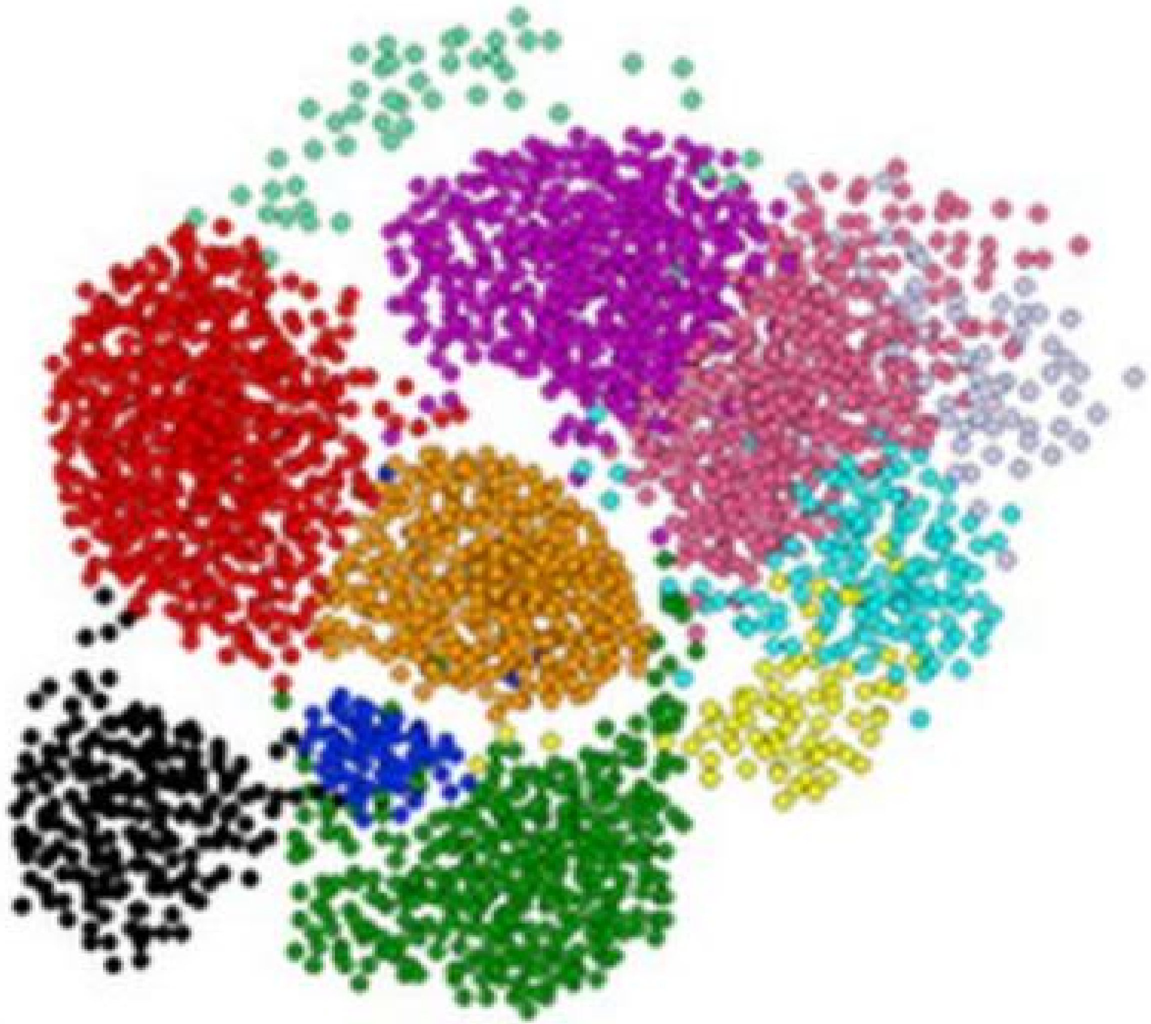
The Problem of Clustering

- Given a **set of points(点集)**, with a notion of **distance** between points, **group the points** into some number of ***clusters(簇)***, so that
  - Members of a cluster are close/similar to each other
  - Members of different clusters are dissimilar
- **Usually:**
  - Points are in a high-dimensional space
  - Similarity is defined using a distance measure
    - Euclidean, Cosine, Jaccard, edit distance, …

Example: Clusters & Outliers



Clustering is a hard problem!



Why is it hard?

- Clustering in two dimensions looks easy
- Clustering small amounts of data looks easy
- And in most cases, looks are not deceiving (欺骗性)

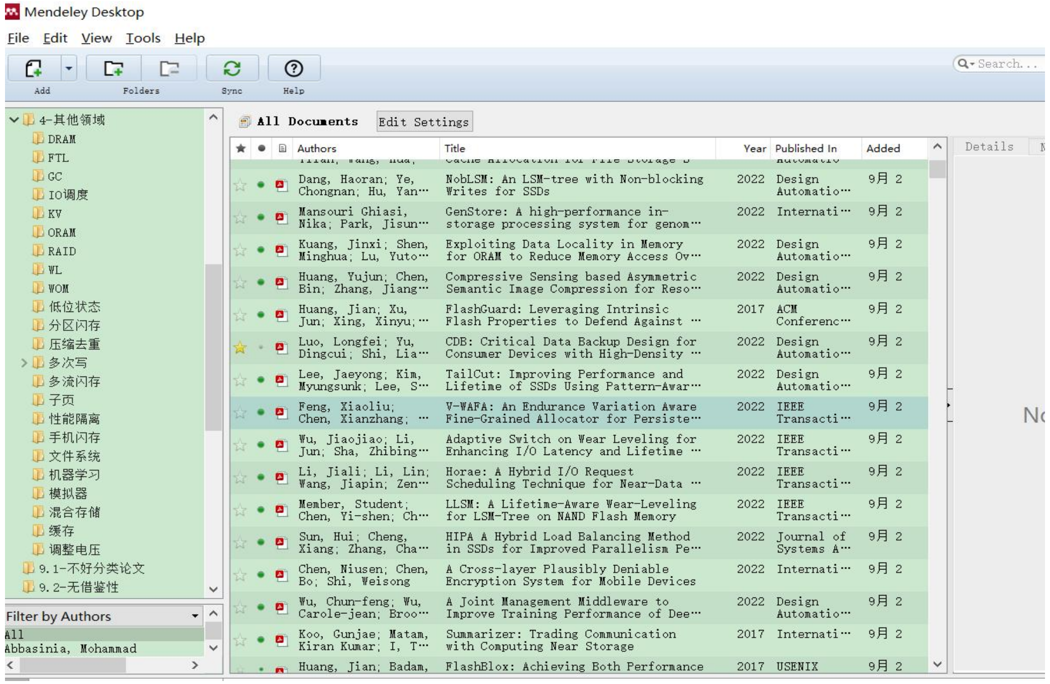
- However, many applications involve not 2, but **10 or 10,000 dimensions**
- **High-dimensional spaces look different:** Almost all pairs of points are at about the same distance

Clustering Problem: Galaxies

- **SkyCat: A catalog of 2 billion "sky objects" represents objects by their radiation in 7 dimensions (frequency bands)**
- **Problem:** Cluster into similar objects, e.g., galaxies (星系), nearby stars (近恒星), quasars (类星体), etc.
- Sloan Digital Sky Survey (斯隆数字化巡天项目)

Clustering Problem: Documents

- Finding topics: Represent a document by a vector $(x_1, x_2, \ldots, x_k)$, where $x_i = 1$ iff the i th word (in some order) appears in the document
  - It actually doesn’ t matter if k is infinite; i.e., we don’ t limit the set of words



- **Documents with similar sets of words may be about the same topic**

Clustering Problem: Music CDs

- **Intuitively: Music divides into categories, and customers prefer a few categories**
  - But what are categories really?

- Represent a CD by a set of customers who bought it:
  - Similar CDs have similar sets of customers, and vice-versa

Clustering Problem: Music CDs

- **Space of all CDs:** Think of a space with one dim. for each customer
  - Values in a dimension may be 0 or 1 only
  - A CD is a point in this space $(x_1, x_2, \ldots, x_k)$, where $x_i = 1$ iff the i^{th} customer bought the CD

- For Amazon, the dimension is tens of millions
- **Task:** Find clusters of similar CDs

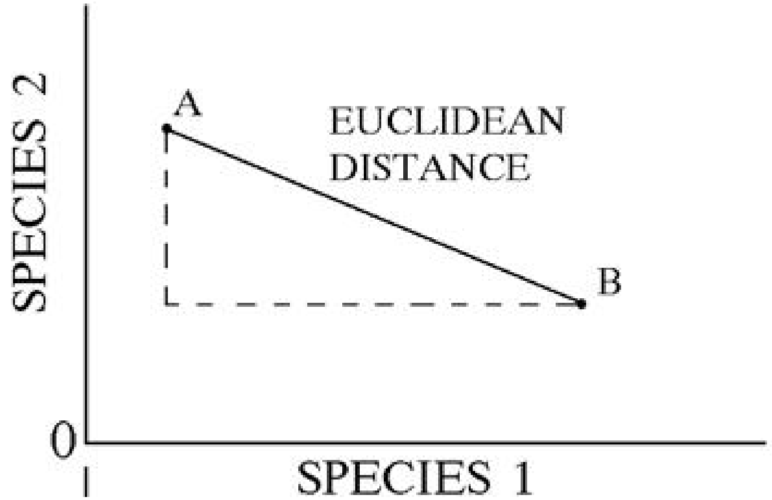
Cosine, Jaccard, and Euclidean

- **As with CDs we have a choice when we think of documents as sets of words or shingles:**
  - **Sets as points:** Measure similarity by **Euclidean distance**
  - **Sets as sets:** Measure similarity by the **Jaccard distance**
  - **Sets as vectors:** Measure similarity by the **Cosine distance**

Euclidean Distance

❑ Euclidean distance(欧氏距离)

➢ 也就是我们通常想象的距离. 在n维欧氏空间下, 每个点是一个n维实数向量. 在该空间下的传统距离测度, 即我们常说的L2范式(L2-norm).



$$d(p,q)=\sqrt{\sum_{j=1}^{d}(p_j-q_j)^2}$$

❑ Euclidean similarity

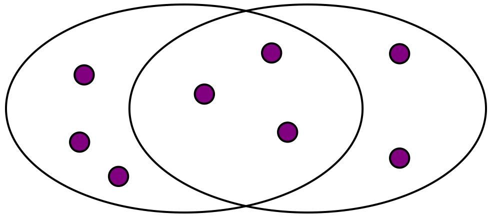
➢ $\frac{1}{1+d(p,q)}$, (0, 1]. closer to 1, the more similar

Jaccard Distance

- **Goal: define what "distance" means in high-dim. space**
  - The **Jaccard similarity** of two **sets** is the size of their intersection(交集) divided by the size of their union(并集):

$$sim(C_1, C_2) = |C_1 \cap C_2| / |C_1 \cup C_2|$$

  - **Jaccard distance:** $d(C_1, C_2) = 1 - |C_1 \cap C_2| / |C_1 \cup C_2|$



3 in intersection
8 in union
Jaccard similarity= 3/8
Jaccard distance = 5/8

Example: Jaccard Distance

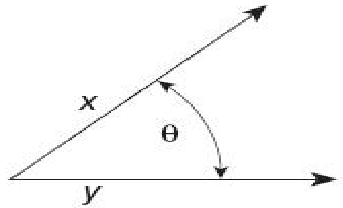
- Example: The Jaccard distance for the documents?

D1	D2	D3	D4
apple releases new ipod	apple releases new ipad	new apple pie recipe	Vefa rereases new book with apple pie recipes

- **Ans:**
  - sim(D1,D2) = 3/5, sim(D1,D3) = sim(D2,D3) = 2/6, sim(D1,D4) = sim(D2,D4) = 3/9
  - d(D1,D2)=2/5, d(D1,D3)=d(D2,D3)=4/6, d(D1,D4)=d(D2,D4)=6/9

Cosine Similarity

- Sim(X,Y) = cos(X,Y)
  - The cosine of the angle between X and Y



Geometric illustration of the cosine measure.

- If the vectors are aligned (correlated) angle is zero degrees and cos(X,Y)=1
- If the vectors are orthogonal (no common coordinates) angle is 90 degrees and cos(X,Y) = 0

- Cosine is commonly used for comparing documents, where we assume that the vectors are normalized by the document length.

Cosine Similarity

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- **Cosine similarity**: $cos(d_1, d_2) = \dfrac{d_1 \bullet d_2}{||d_1||\ ||d_2||}$
  - d1 and d2 are two vectors. • indicates vector dot product (向量的点积, 或称内积); ||d|| is the length of vector d (向量的大小).
  - (-1,1). closer to 1, the more similar

- Example: d_1 = **3 2 0 5 0 0 0 2 0 0 ,** d_2 = **1 0 0 0 0 0 0 1 0 2**
- **Ans:**
  - First, d1 • d2= 3*1+2*0+0*0+5*0+0*0+0*0+0*0+2*1+0*0+0*2=5;
  - ||d1||=$\sqrt{3*3+2*2+0*0+5*5+0*0+0*0+0*0+2*2+0*0+0*0}$=6.481;
  - ||d2||= $\sqrt{1*1+0*0+0*0+0*0+0*0+0*0+0*0+1*1+0*0+2*2}$=2.245.
  - So, cos(d1, d2)=0.3150

Cosine Distance

- **Cosine Distance(余弦距离)**: $dis(d_1, d_2) = 1 - cos(d_1, d_2)$
  - (0,2)
  - closer to 0, the more similar

Example: Cosine Distance

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- Example: The cosine distance for the documents?

document	Apple	Microsoft	Obama	Election
D1	10	20	0	0
D2	30	60	0	0
D3	60	30	0	0
D4	0	0	10	20

- **Ans:**

dis(D1,D2) =0 → D1 and D2 similarity

dis (D3,D1) = dis (D3,D2) = 1/5

dis(D4,D1) = dis(D4,D2) = dis(D4,D3) = 1 → D4 and D1 dissimilarity;

补充: 编辑距离

- **Edit Distance(编辑距离):** The edit distance between two strings $x = x_1x_2 \ldots x_n$ and $y = y_1y_2 \ldots y_m$ is the smallest number of insertions and deletions of single characters that will convert x to y.
  - This distance makes sense when points are strings (编辑距离适用于字符串比较).

- **Example:** What is the edit distance between the strings x = abcde and y =acfdeg?
- **Ans**: d(x, y) = 3. To convert x to y: Step 1. Delete b; Step 2: Insert f after c; Step 3: Insert g after e. No sequence of fewer than three insertions and/or deletions will convert x to y.

补充: 编辑距离

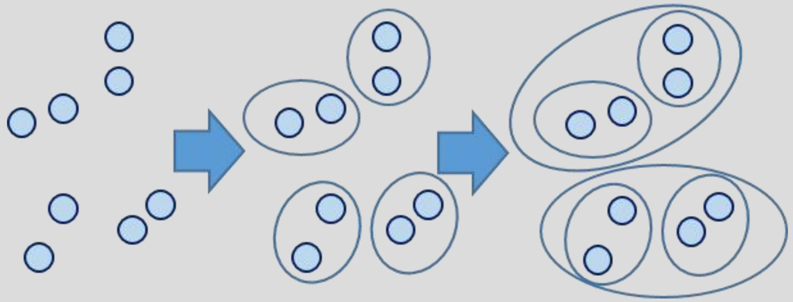
- **Longest common subsequence (LCS, 最长公共子序列)** of x and y is a string that is constructed by deleting positions from x and y, and that is as long as any string that can be constructed that way.
- Then, edit distance d(x, y)=the length of x +the length of y - 2* the length of their LCS.

- **Example:** What is the edit distance between the strings x = abcde and y =acfdeg?
- **Ans**: d(x, y) = 3. LCS is "acde". Then 5+6-2*4=3.

补充: 海明距离

- **Hamming Distance(海明距离):** Given a space of vectors, we define the Hamming distance between two vectors to be the number of components in which they differ.

- **Example**: What is the Hamming distance between the vectors 10101 and 11110
- **Ans**: Hamming distance is 3. That is, these vectors differ in the second, fourth, and fifth components (10101 and 11110), while they agree in the first and third components.



Section 5.2: Hierarchical clustering

Clustering Overview

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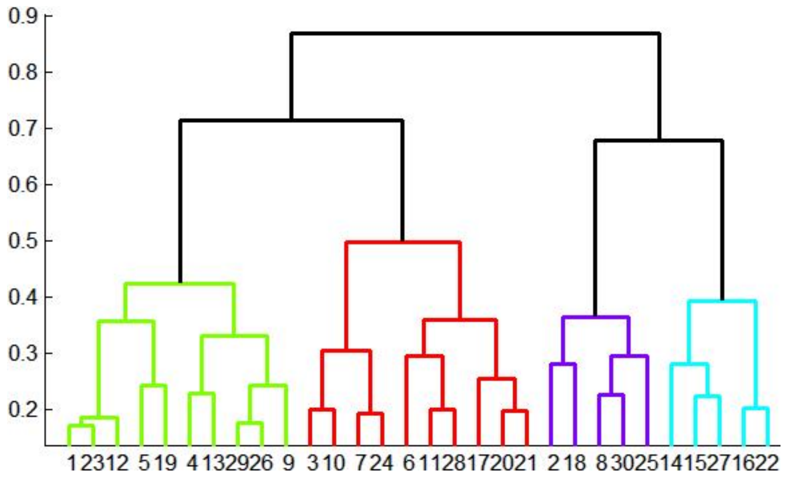
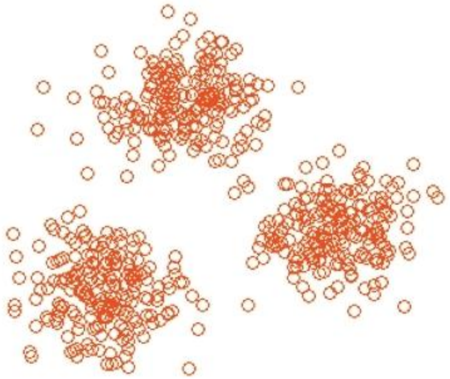
❑Methods of clustering:

❑1、Hierarchical(层次聚类, 分级聚类, 凝聚式算法):



- ➢**Agglomerative** (bottom up):
  - Initially, each point is a cluster
  - Repeatedly combine the two "nearest" clusters into one
- ➢**Divisive** (top down):
  - Start with one cluster and recursively split it

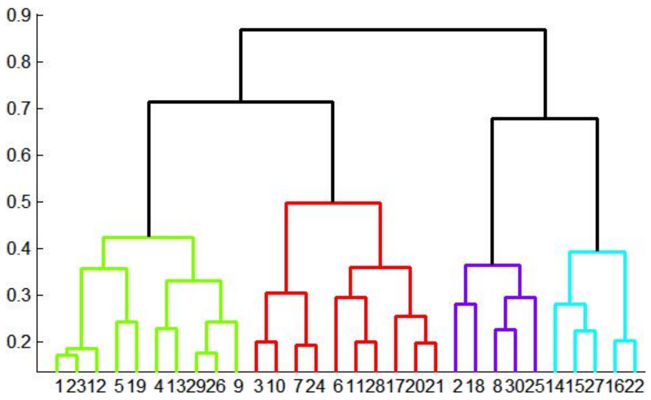
❑2、Point assignment(点分配):



- ➢Maintain a set of clusters
- ➢Points belong to "nearest" cluster
- ➢e.g. K-mean, BFR, CURE…

Hierarchical Clustering

- **Key operation:** **Repeatedly combine two nearest clusters**



- **Three important questions:**
  - **1)** How do you represent a cluster of more than one point?
  - **2)** How do you determine the "nearness" of clusters?
  - **3)** When to stop combining clusters?