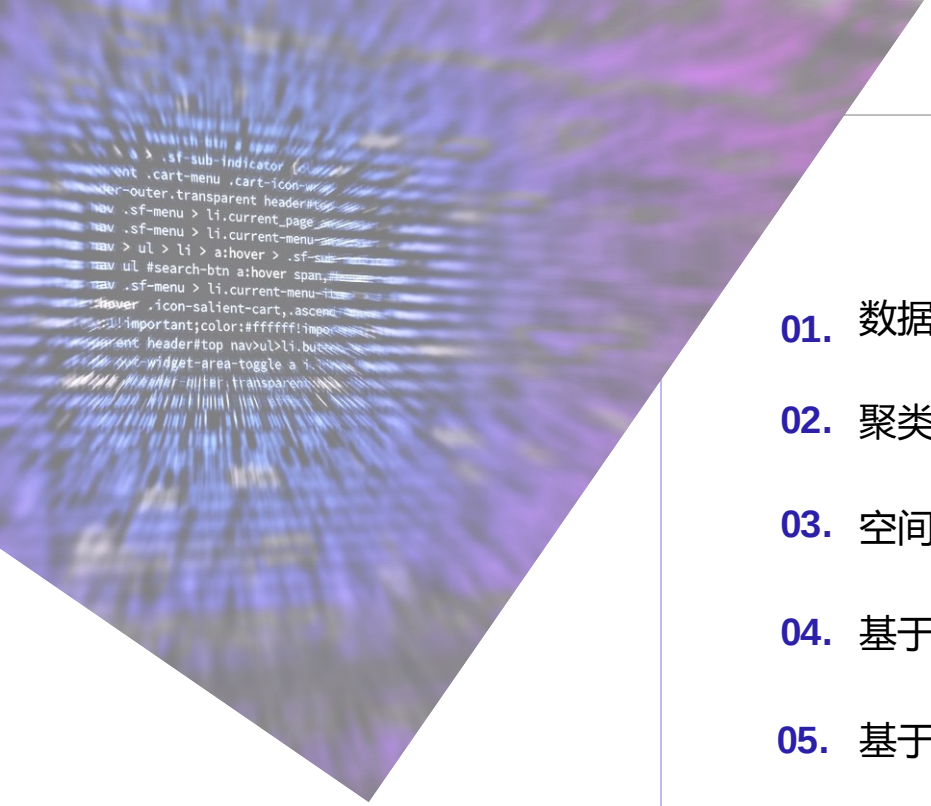
机器学习导论

第10章 聚类

谢茂强

南开大学软件学院

本章部分内容来自于吴恩达Coursera网课



目录

01. 数据分析与聚类简介

02. 聚类性能评价指标

03. 空间和距离（相似度）度量

04. 基于划分的聚类 (K-Means, GMM)

05. 基于密度的聚类 (DBSCAN)

06. 层次聚类方法 (AGNES)

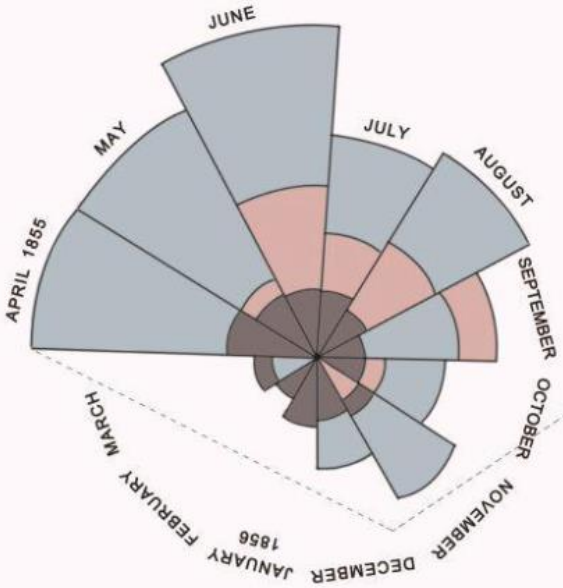
07. 聚类可视化

DIAGRAM OR THE CAUSES OR MORTALITY

IN THE ARMY IN THE EAST

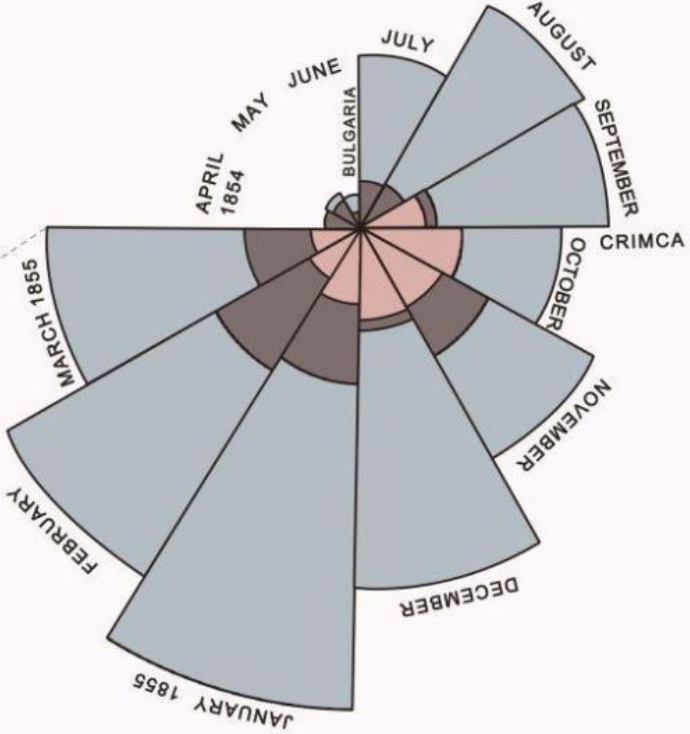
2.

APRIL 1855 TO MARCH 1856



1.

APRIL 1854 TO MARCH 1855



The Areas of the blue, red, & black wedges are each measured from the centre as the common vertex.

The blue wedges measured from the centre of the circle represent area for area, the deaths from Preventible or Mitigable Zymotic diseases, the red wedges measured from the centre the deaths from wounds, & the black wedges measured from the centre the deaths from all other causes

The black line across the red triangle in Nov.r 1854 marks the boundary of the deaths from all other causes during the month.

In October 1854, & April 1855, the black area coincides with the red, in January & February 1856, the blue coincides with the black.

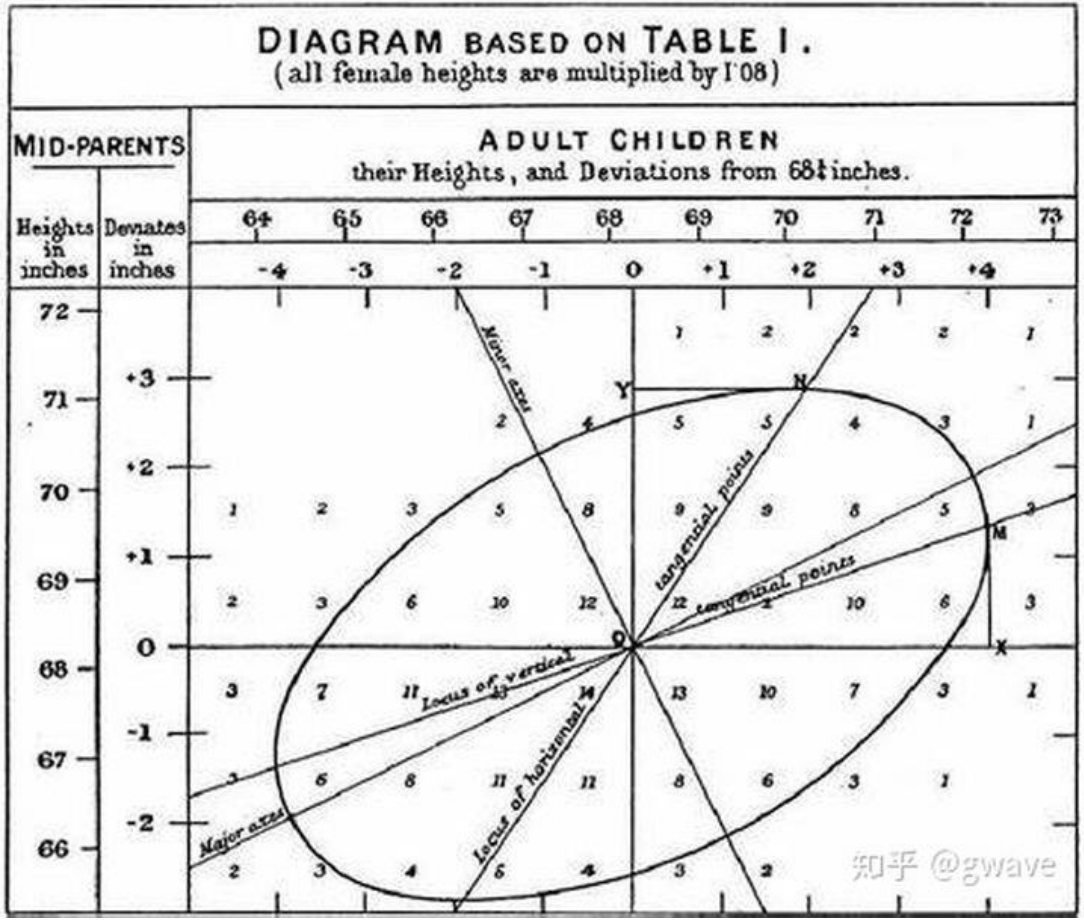


DIAGRAM BASED ON TABLE I.
(all female heights are multiplied by 1·08)
MID-PARENTS
Heights in inches
Deviates in inches
ADULT CHILDREN
their Heights, and Deviations from 68½ inches.
64 65 66 67 68 69 70 71 72 73
-4 -3 -2 -1 0 +1 +2 +3 +4
72 71 70 69 68 67 66
+3 +2 +1 0 -1 -2
Minor axes
tangential points
tangential points
Locus of vertical
Locus of horizontal
Major axes
Y
N
M
X
O
知乎 @gwave

聚类：一种无监督学习算法

聚类目标: 对数据集进行聚合,使形成一些簇（类），用以了解数据（分布）的内在性质及规律

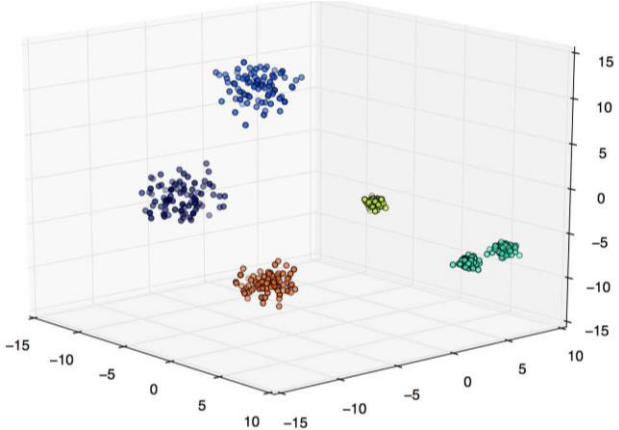
聚类原则: 物以类聚

聚类结果: 相似的归为一类

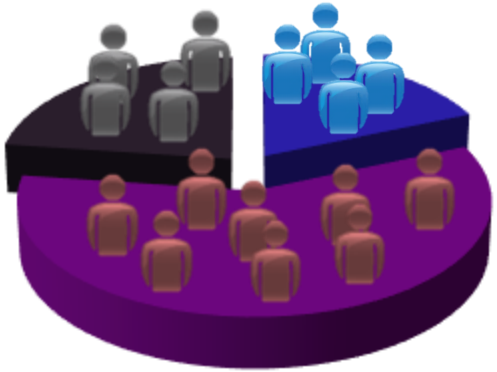
地　　位: 了解数据分布的重要工具，是后续分析的重要基础

示　　例:

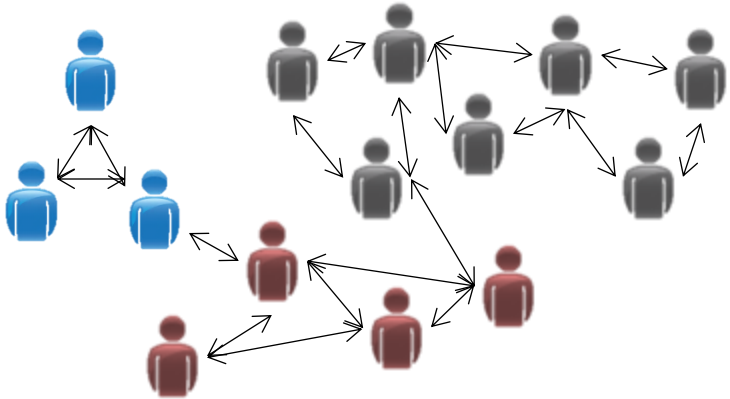
根据客户的特征进行类别划分



聚类的应用



Market segmentation



Social network analysis

Organize computing clusters

Image credit: NASA/JPL-Caltech/E. Churchwell (Univ. of Wisconsin, Madison)

Astronomical data analysis

1. 聚类的输入输出定义

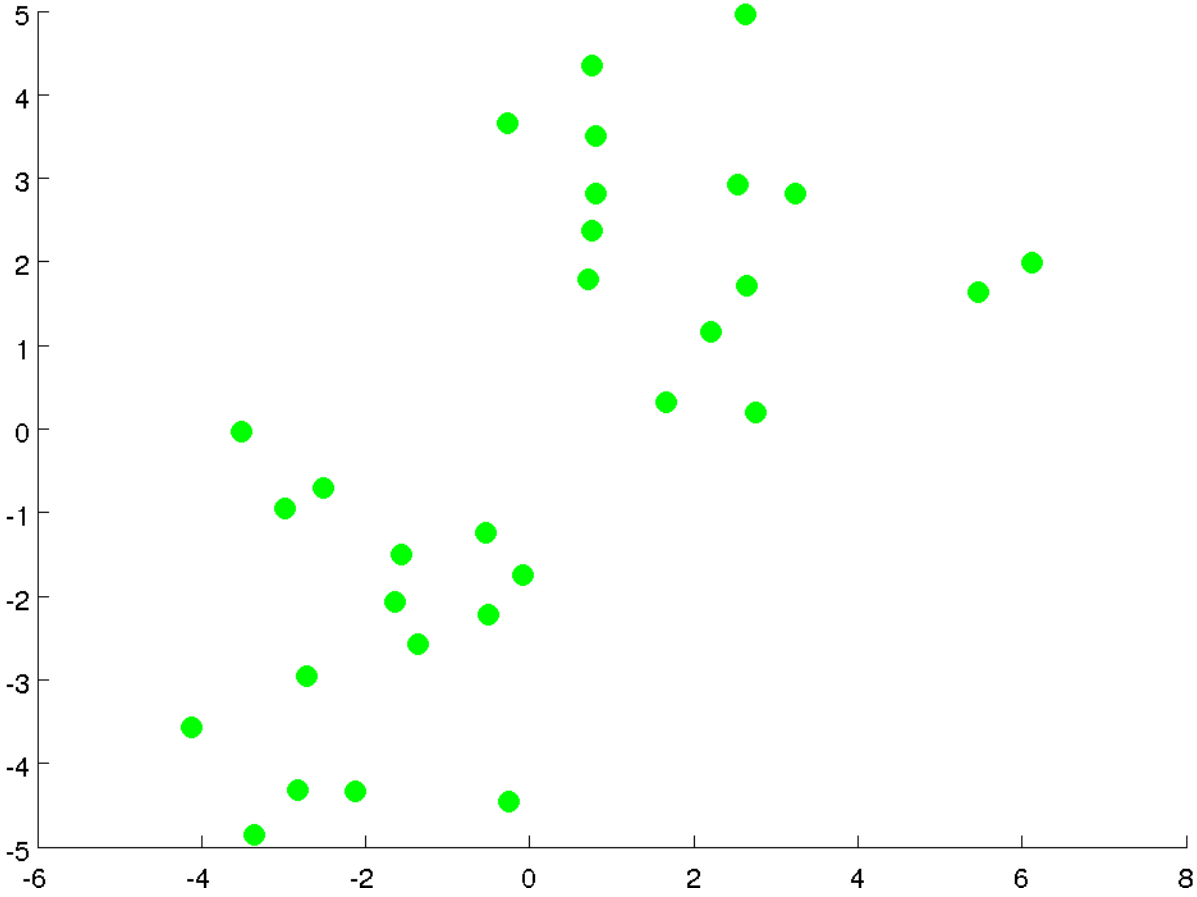
输入： $D = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_m\}$ $\boldsymbol{x}_i = (x_{i1}; x_{i2}; \cdots; x_{in})$

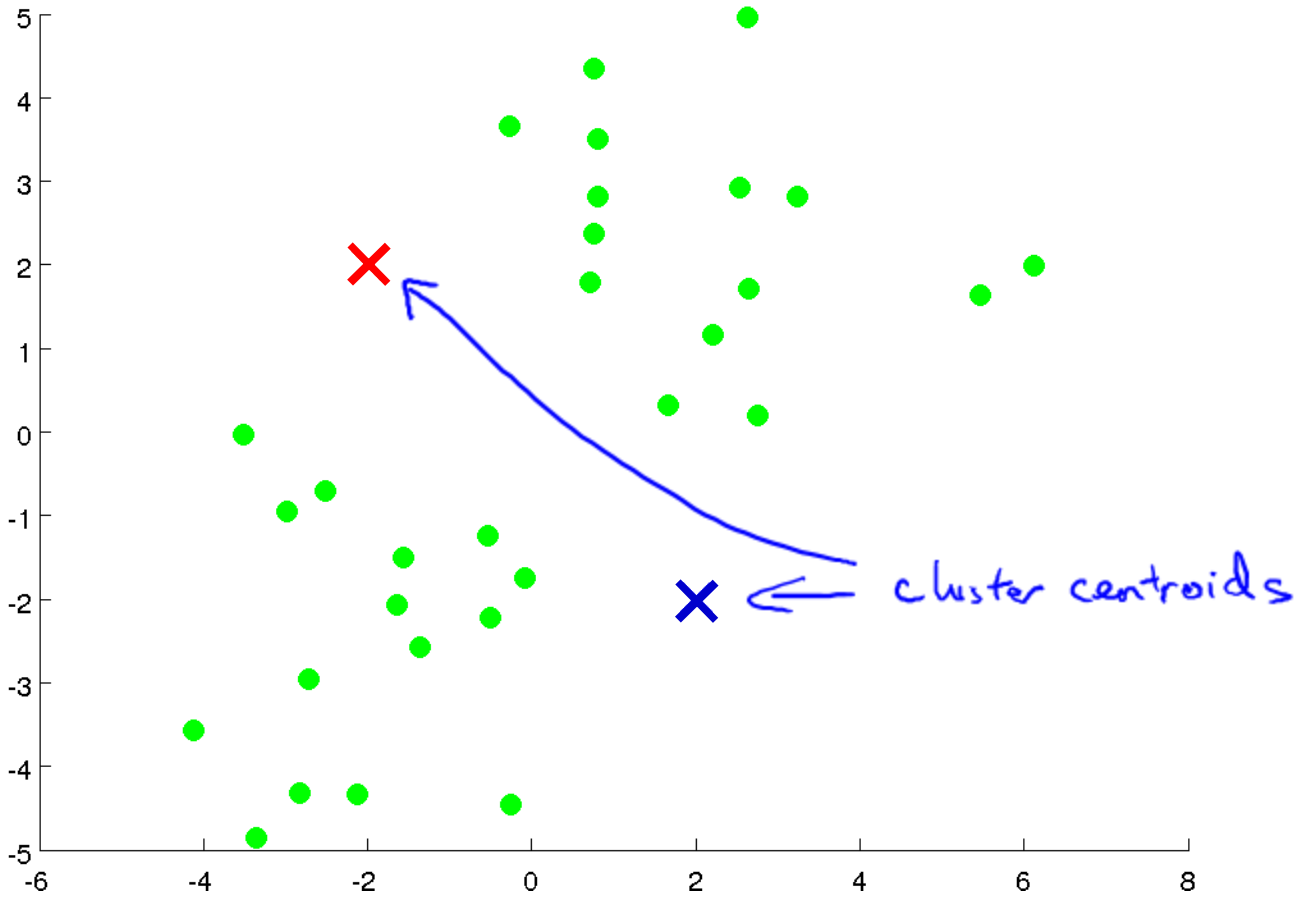
输出： $\boldsymbol{x} \in C_l$ 簇集合： $\{C_l \mid l = 1, 2, \cdots, k\}$

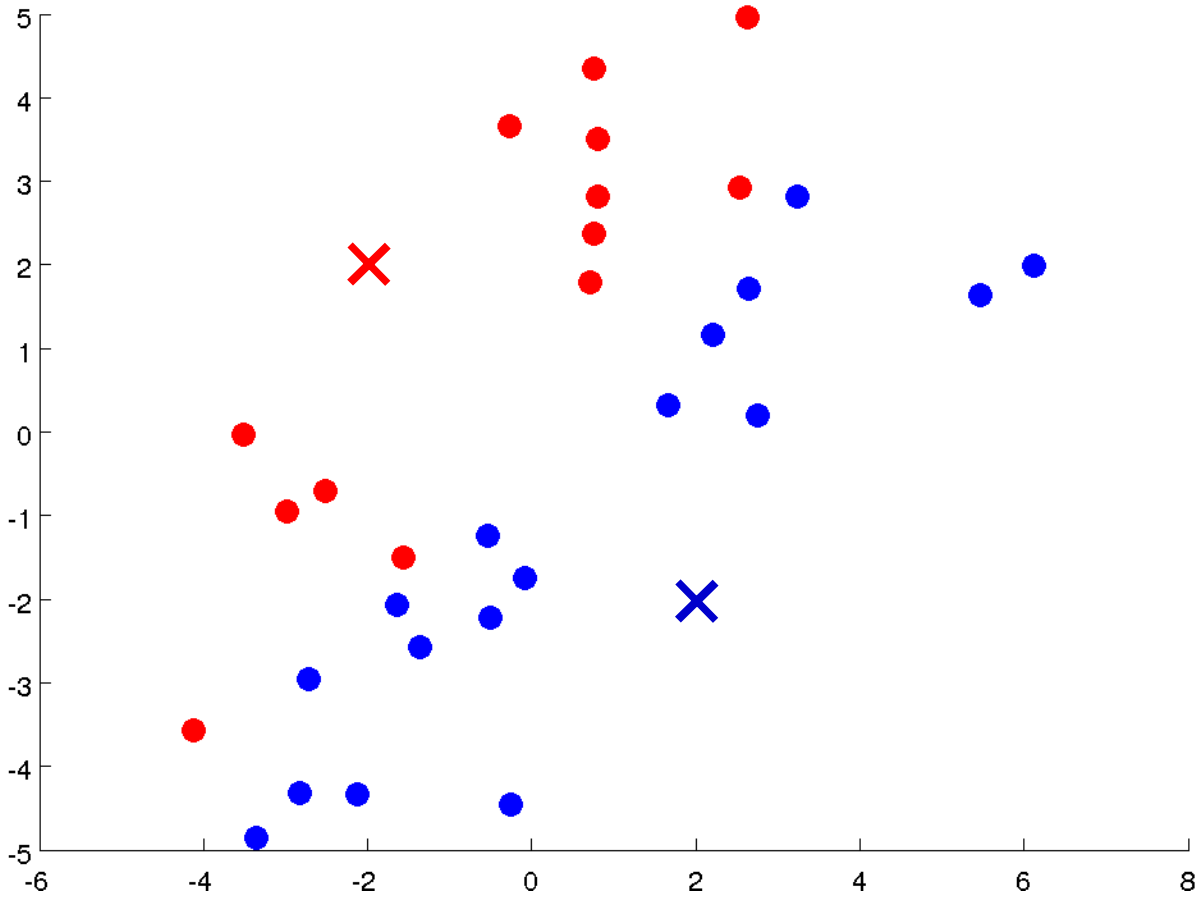
$C_{l'} \cap_{l' \neq l} C_l = \varnothing$ $D = \cup_{l=1}^{k} C_l$

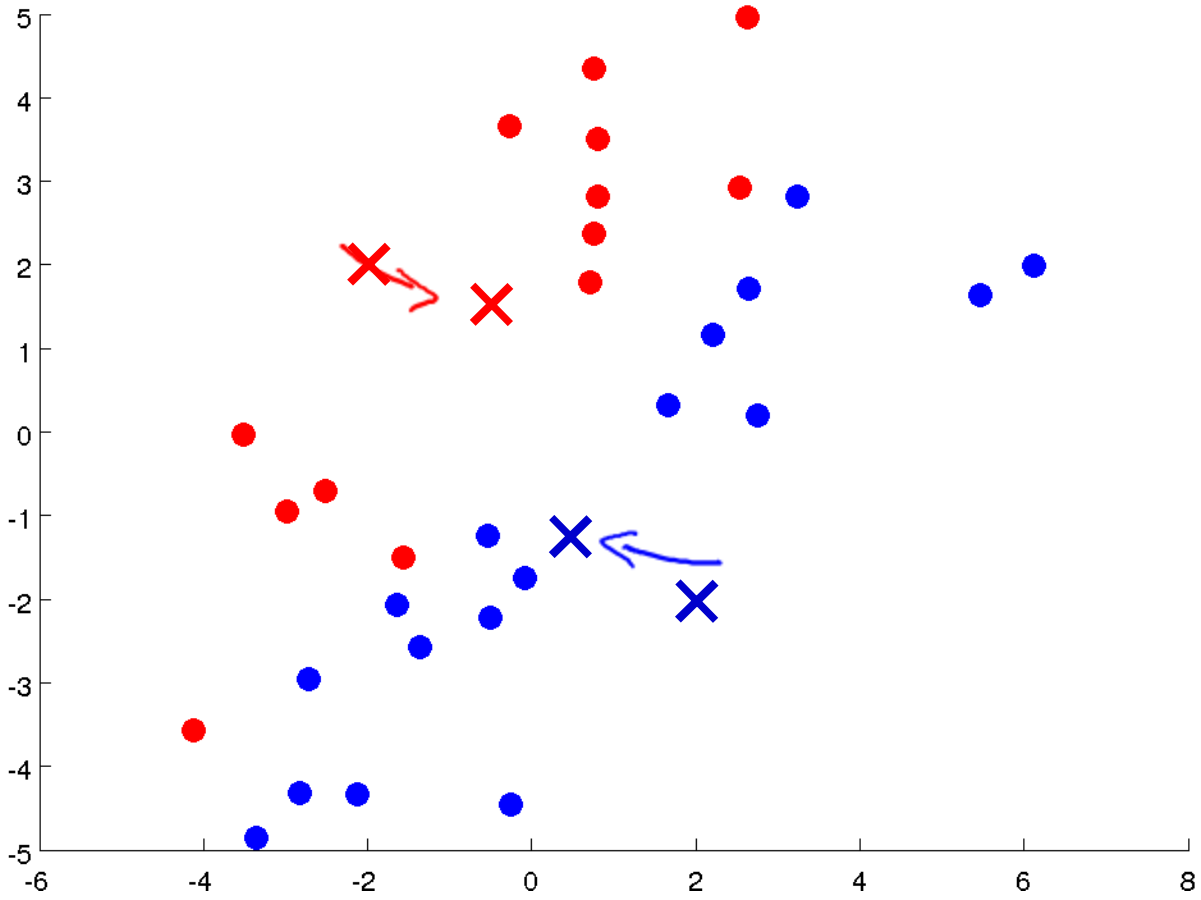
聚类中一种算法思路的示意（下页开始）

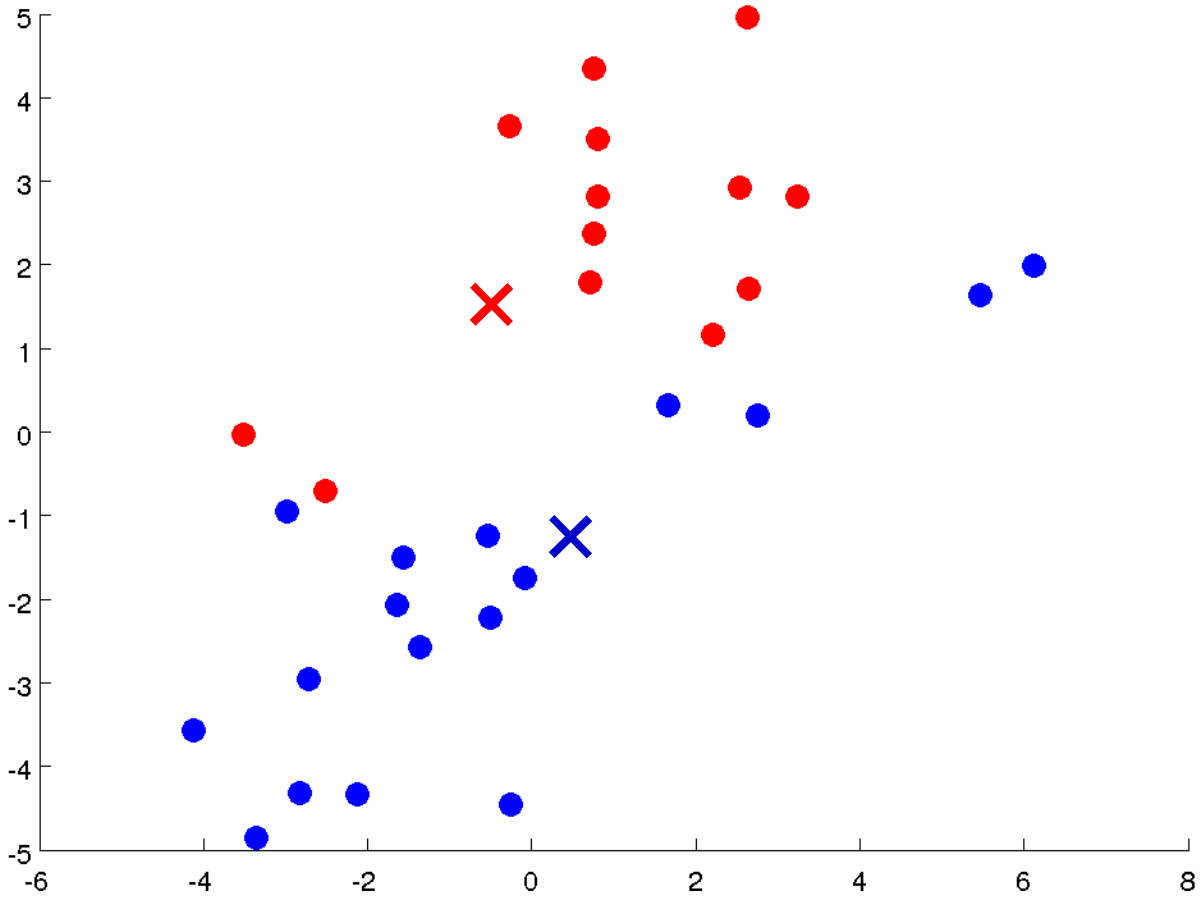
周志华 .《机器学习》 Chpt. 9. P197

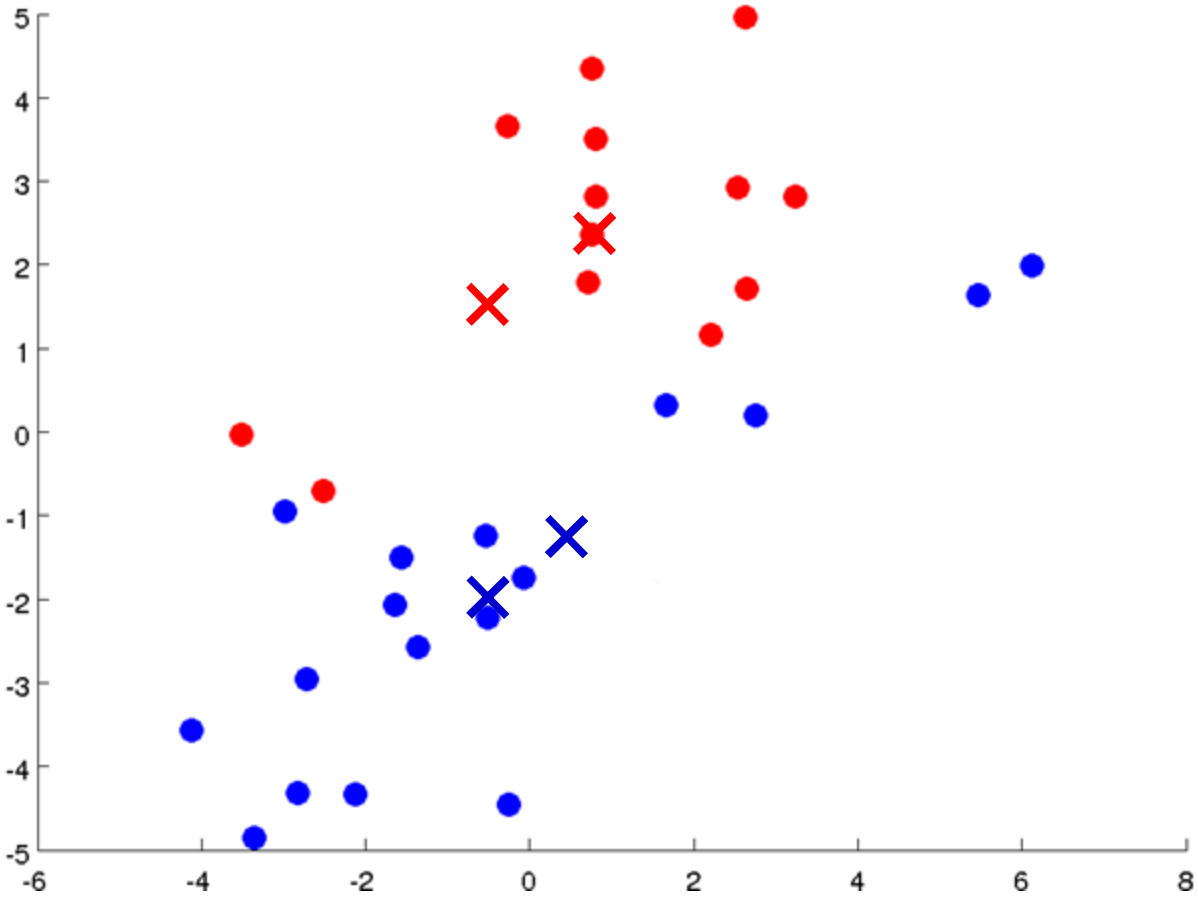

5
4
3
2
1
0
-1
-2
-3
-4
-5
-6
-4
-2
0
2
4
6
8

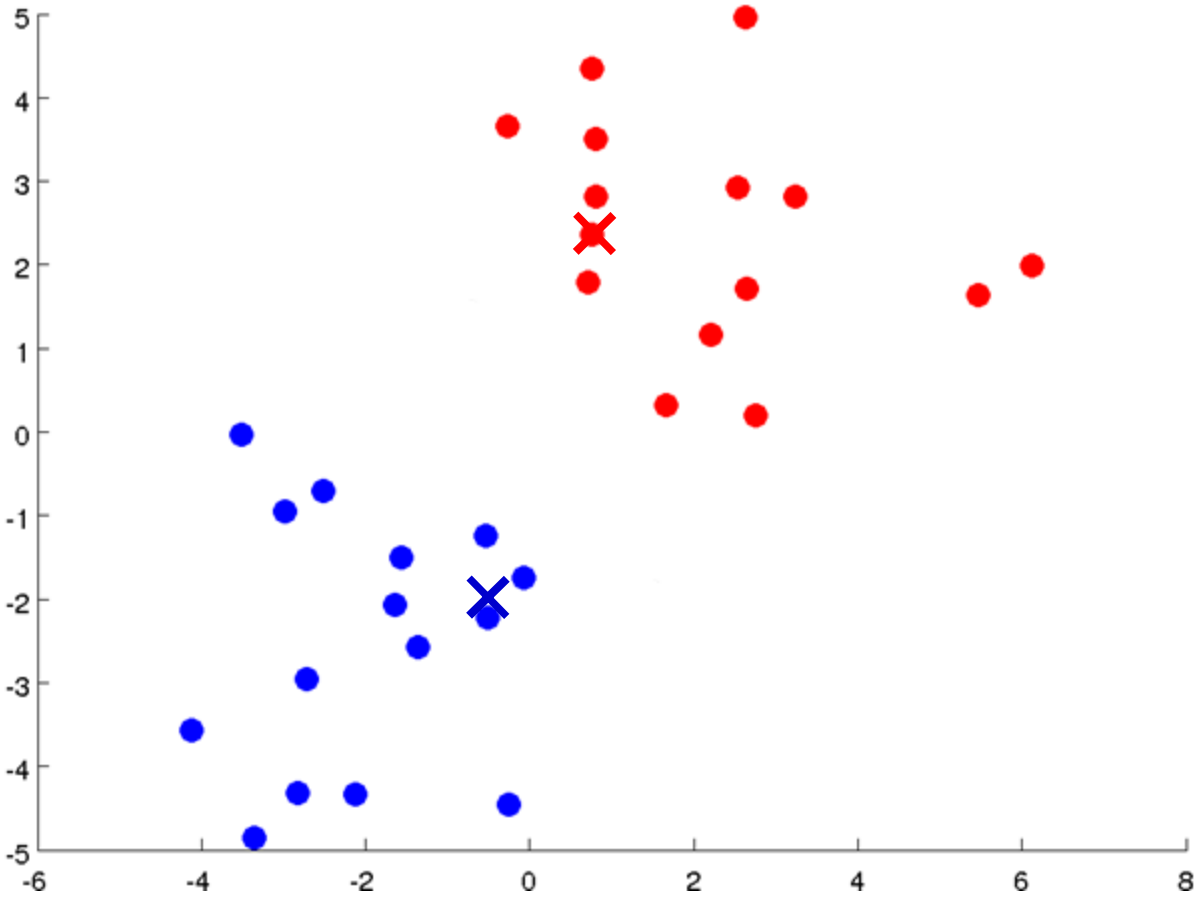

5
4
3
2
1
0
-1
-2
-3
-4
-5
-6
-4
-2
0
2
4
6
8
cluster centroids

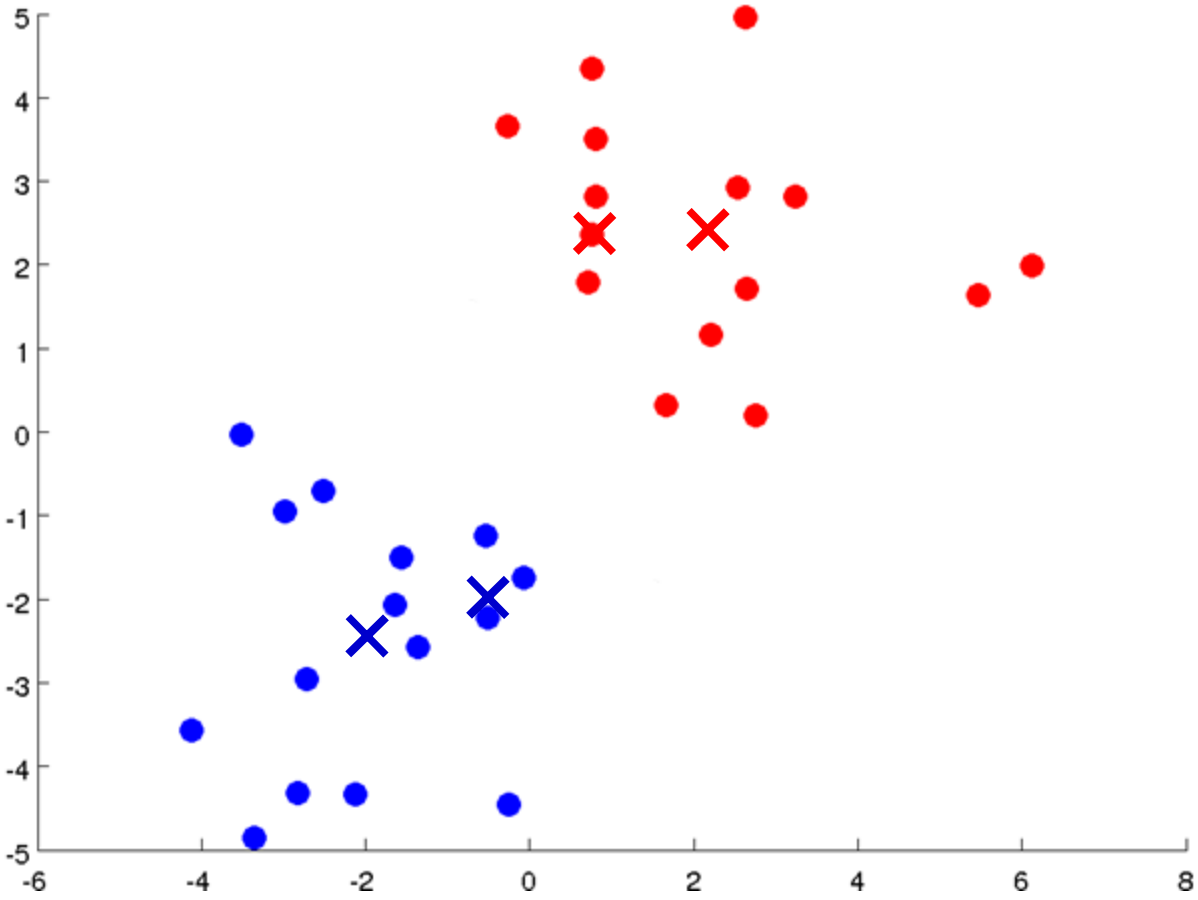

5
4
3
2
1
0
-1
-2
-3
-4
-5
-6
-4
-2
0
2
4
6
8

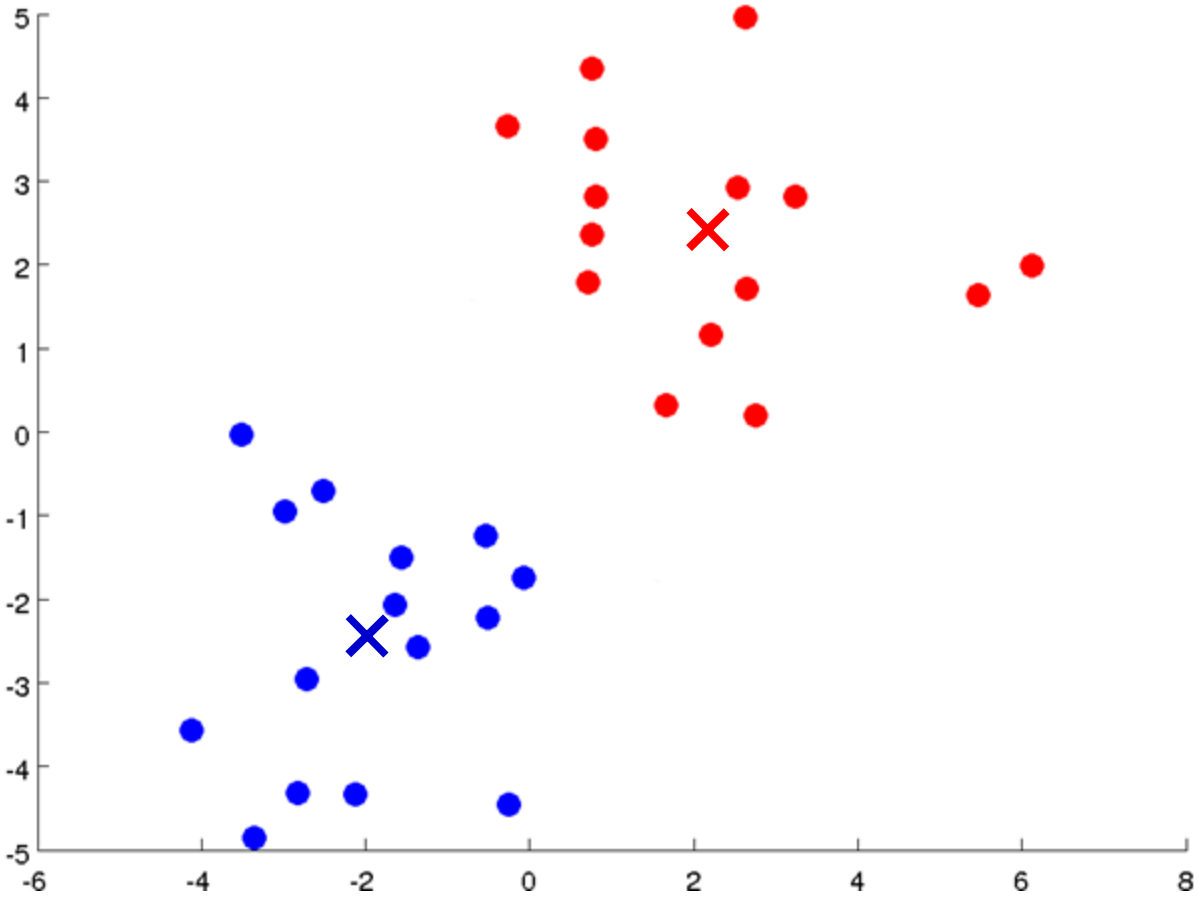

5
4
3
2
1
0
-1
-2
-3
-4
-5
-6
-4
-2
0
2
4
6
8


5
4
3
2
1
0
-1
-2
-3
-4
-5
-6
-4
-2
0
2
4
6
8


5
4
3
2
1
0
-1
-2
-3
-4
-5
-6
-4
-2
0
2
4
6
8


5
4
3
2
1
0
-1
-2
-3
-4
-5
-6
-4
-2
0
2
4
6
8


5
4
3
2
1
0
-1
-2
-3
-4
-5
-6
-4
-2
0
2
4
6
8


5
4
3
2
1
0
-1
-2
-3
-4
-5
-6
-4
-2
0
2
4
6
8

2. 聚类的性能指标

- 聚类性能指标（有效性指标，validity index），用来评价结果，进而作为优化目标。（物以类聚）

外部指标（External Index）

与某个“参考模型”进行比较

比如专家标注的簇标签

内部指标（Internal Index）

簇内相似度（intra-cluster sim）高

簇间相似度（inter-cluster sim）低

类内距、方差 …

2.1 聚类性能的外部指标 (从“样本对”归属的角度)

对数据集 $D=\{\boldsymbol{x}_1,\boldsymbol{x}_2,\ldots,\boldsymbol{x}_m\}$, 假定通过聚类给出的簇划分为 $\mathcal{C}=\{C_1, C_2,\ldots,C_k\}$, 参考模型给出的簇划分为 $\mathcal{C}^*=\{C_1^*,C_2^*,\ldots,C_s^*\}$. 相应地, 令 $\boldsymbol{\lambda}$ 与 $\boldsymbol{\lambda}^*$ 分别表示与 $\mathcal{C}$ 和 $\mathcal{C}^*$ 对应的簇标记向量. 我们将样本两两配对考虑, 定义

$$a=|SS|,\quad SS=\{(\boldsymbol{x}_i,\boldsymbol{x}_j)\mid \lambda_i=\lambda_j,\lambda_i^*=\lambda_j^*,i<j)\},\tag{9.1}$$

$$b=|SD|,\quad SD=\{(\boldsymbol{x}_i,\boldsymbol{x}_j)\mid \lambda_i=\lambda_j,\lambda_i^*\neq\lambda_j^*,i<j)\},\tag{9.2}$$

$$c=|DS|,\quad DS=\{(\boldsymbol{x}_i,\boldsymbol{x}_j)\mid \lambda_i\neq\lambda_j,\lambda_i^*=\lambda_j^*,i<j)\},\tag{9.3}$$

$$d=|DD|,\quad DD=\{(\boldsymbol{x}_i,\boldsymbol{x}_j)\mid \lambda_i\neq\lambda_j,\lambda_i^*\neq\lambda_j^*,i<j)\},\tag{9.4}$$

其中集合 SS 包含了在 $\mathcal{C}$ 中隶属于相同簇且在 $\mathcal{C}^*$ 中也隶属于相同簇的样本对, 集合 SD 包含了在 $\mathcal{C}$ 中隶属于相同簇但在 $\mathcal{C}^*$ 中隶属于不同簇的样本对, ……由于每个样本对 $(\boldsymbol{x}_i,\boldsymbol{x}_j)$ $(i<j)$ 仅能出现在一个集合中, 因此有 $a+b+c+d=m(m-1)/2$ 成立.

2.1聚类性能的外部指标

- Jaccard系数 (Jaccard Index, Jaccard Similarity Coefficient)

$$JC = \frac{a}{a+b+c}$$

- FM指数（Fowlkers & Mallows Index, FMI）

$$FMI = \sqrt{\frac{a}{a+b} \cdot \frac{a}{a+c}}$$

- Rand指数（Rand Index, RI）

$$RI = \frac{2(a+d)}{m(m-1)}$$

		Groundtruth	
		同簇	异簇
Prediction	同簇	SS(a)	SD(b)
	异簇	DS(c)	DD(d)

2.2 聚类性能的内部指标

- 簇C内样本间平均距离

$$\operatorname{avg}(C) = \frac{2}{|C|(|C|-1)} \sum_{1 \leqslant i < j \leqslant |C|} \operatorname{dist}(\boldsymbol{x}_i, \boldsymbol{x}_j) \ , \tag{9.8}$$

- 簇C内样本间最远距离

$$\operatorname{diam}(C) = \max_{1 \leqslant i < j \leqslant |C|} \operatorname{dist}(\boldsymbol{x}_i, \boldsymbol{x}_j) \ , \tag{9.9}$$

2.2 聚类性能的内部指标

- 簇间距离

$$d_{\min}(C_i, C_j) = \min_{\boldsymbol{x}_i \in C_i, \boldsymbol{x}_j \in C_j} \operatorname{dist}(\boldsymbol{x}_i, \boldsymbol{x}_j) \ , \tag{9.10}$$

$$d_{\mathrm{cen}}(C_i, C_j) = \operatorname{dist}(\boldsymbol{\mu}_i, \boldsymbol{\mu}_j) \ , \tag{9.11}$$

- DB指数(Davies-Bouldin Index, DBI)

$$\mathrm{DBI} = \frac{1}{k} \sum_{i=1}^{k} \max_{j \neq i} \left(\frac{\operatorname{avg}(C_i) + \operatorname{avg}(C_j)}{d_{\mathrm{cen}}(\boldsymbol{\mu}_i, \boldsymbol{\mu}_j)} \right) \ . \tag{9.12}$$

DBI越小聚类性能越好

2.2 聚类性能的内部指标

- 簇间距离

$$d_{\min}(C_i, C_j) = \min_{\boldsymbol{x}_i \in C_i, \boldsymbol{x}_j \in C_j} \operatorname{dist}(\boldsymbol{x}_i, \boldsymbol{x}_j) \ , \tag{9.10}$$

$$d_{\mathrm{cen}}(C_i, C_j) = \operatorname{dist}(\boldsymbol{\mu}_i, \boldsymbol{\mu}_j) \ , \tag{9.11}$$

- Dunn指数(Dunn Index, DI)

$$\mathrm{DI} = \min_{1 \leqslant i \leqslant k} \left\{ \min_{j \neq i} \left(\frac{d_{\min}(C_i, C_j)}{\max_{1 \leqslant l \leqslant k} \operatorname{diam}(C_l)} \right) \right\} \ . \tag{9.13}$$

DI越大聚类性能越好

3. 距离度量

- 非负性： $\mathrm{dist}(\boldsymbol{x}_i, \boldsymbol{x}_j) \geqslant 0$
- 同一性： $\mathrm{dist}(\boldsymbol{x}_i, \boldsymbol{x}_j) = 0$ 当且仅当 $\boldsymbol{x}_i = \boldsymbol{x}_j$
- 对称性： $\mathrm{dist}(\boldsymbol{x}_i, \boldsymbol{x}_j) = \mathrm{dist}(\boldsymbol{x}_j, \boldsymbol{x}_i)$
- 三角不等式： $\mathrm{dist}(\boldsymbol{x}_i, \boldsymbol{x}_j) \leqslant \mathrm{dist}(\boldsymbol{x}_i, \boldsymbol{x}_k) + \mathrm{dist}(\boldsymbol{x}_k, \boldsymbol{x}_j)$

3. 距离度量

- 明氏距离(Minkowski distance, L_p 范数)：

$$\mathrm{dist}_{\mathrm{mk}}(\boldsymbol{x}_i, \boldsymbol{x}_j) = \left(\sum_{u=1}^{n} |x_{iu} - x_{ju}|^p \right)^{\frac{1}{p}}$$

- 欧氏距离(Euclidean distance)：

$$\mathrm{dist}_{\mathrm{ed}}(\boldsymbol{x}_i, \boldsymbol{x}_j) = ||\boldsymbol{x}_i - \boldsymbol{x}_j||_2 = \sqrt{\sum_{u=1}^{n} |x_{iu} - x_{ju}|^2}$$

- 曼哈顿距离(Manhattan/City block distance)：

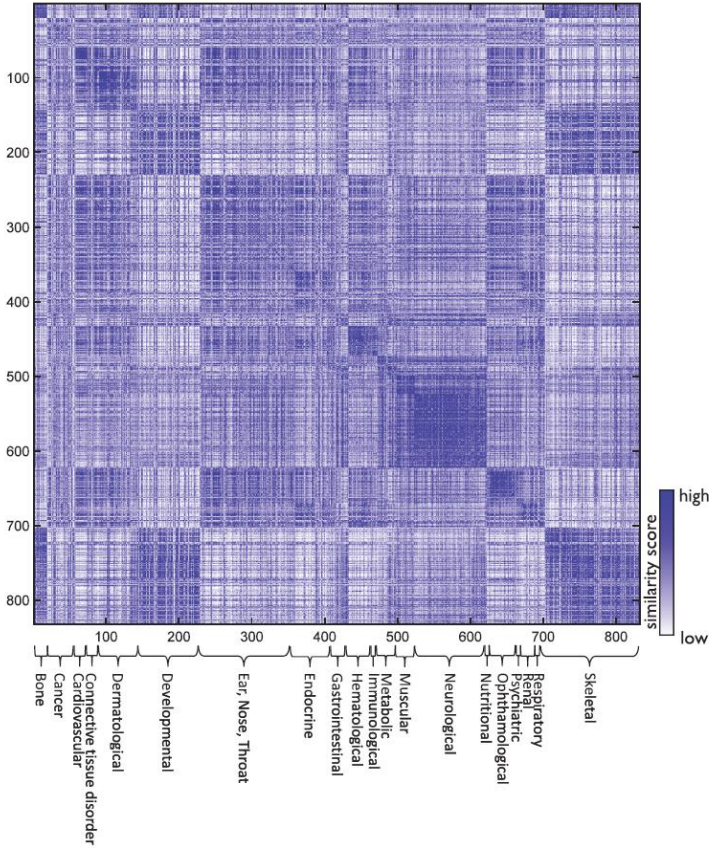
$$\mathrm{dist}_{\mathrm{man}}(\boldsymbol{x}_i, \boldsymbol{x}_j) = ||\boldsymbol{x}_i - \boldsymbol{x}_j||_1 = \sum_{u=1}^{n} |x_{iu} - x_{ju}|$$

3. 距离和空间的关系

- 距离是定义在空间定义之上，是空间的附属
- 常见的空间问题
  - 尺度伸缩
  - 球面距离
  - 流形（manifold）

距离、相似度

示例：可以使用Jaccard Index 作为语义相似度度量



4. 基于划分的K-Means算法

K-means algorithm

Randomly initialize K cluster centroids $\mu_1, \mu_2, \ldots, \mu_K \in \mathbb{R}^n$

Repeat {

for i = 1 to m

$c^{(i)}$:= index (from 1 to K) of cluster centroid closest to $x^{(i)}$

for k = 1 to K

μ_k := average (mean) of points assigned to k cluster

}

4. K-Means算法的优化目标

给定样本集 $D=\{\boldsymbol{x}_1,\boldsymbol{x}_2,\ldots,\boldsymbol{x}_m\}$, “$k$ 均值” (k-means)算法针对聚类所得簇划分 $\mathcal{C}=\{C_1,C_2,\ldots,C_k\}$ 最小化平方误差

$$E=\sum_{i=1}^{k}\sum_{\boldsymbol{x}\in C_i}||\boldsymbol{x}-\boldsymbol{\mu}_i||_2^2\ , \tag{9.24}$$

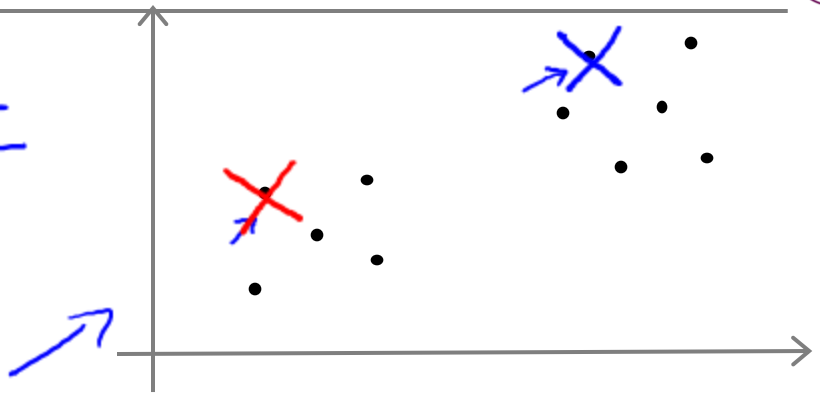
其中 $\boldsymbol{\mu}_i=\frac{1}{|C_i|}\sum_{\boldsymbol{x}\in C_i}\boldsymbol{x}$ 是簇 C_i 的均值向量. 直观来看, 式(9.24) 在一定程度上刻画了簇内样本围绕簇均值向量的紧密程度, E 值越小则簇内样本相似度越高.

簇中心的随机初始化

Should have $K < m$

$K=2$

Randomly pick K training examples.

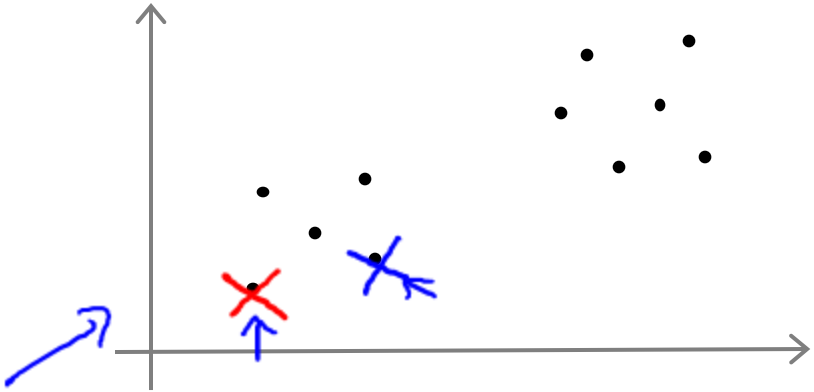


Set $\mu_1, \ldots, \mu_K$ equal to these K examples.

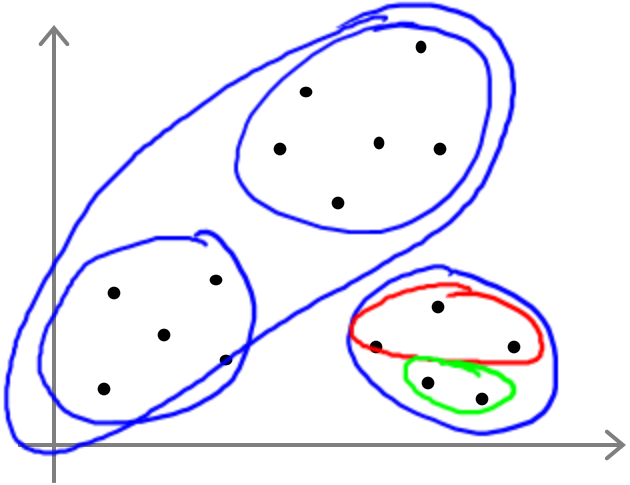
$\mu_1 = x^{(i)}$

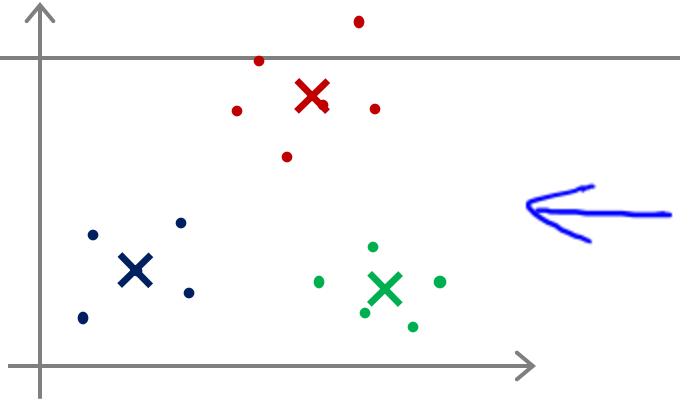
$\mu_2 = x^{(j)}$

$\vdots$

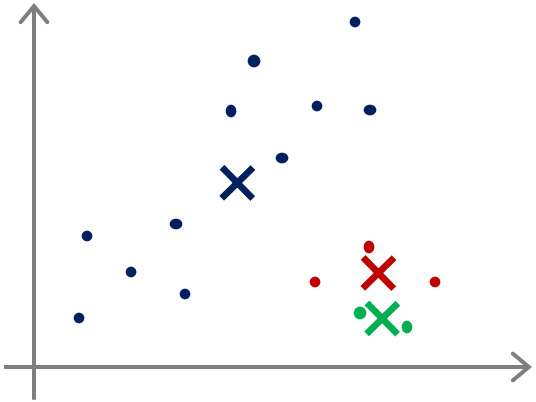


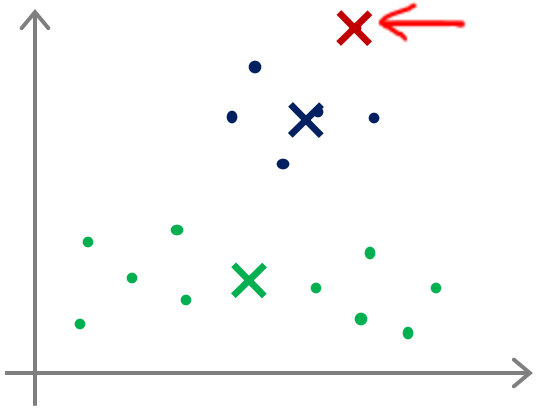
K-Means算法的局部收敛结果





$$J(c^{(1)},\dots,c^{(m)},\mu_1,\dots,\mu_K)$$





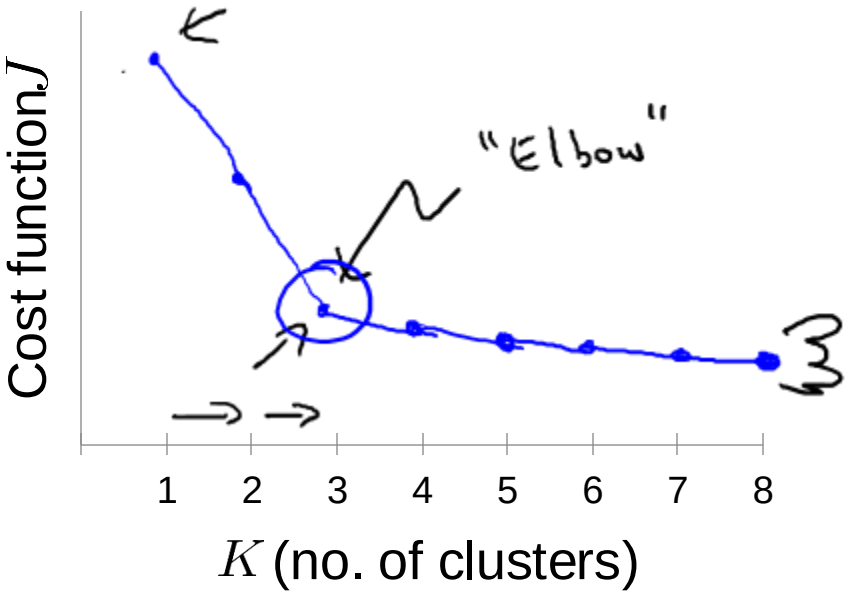
通过多次随机初始化解决陷入局部极值的问题

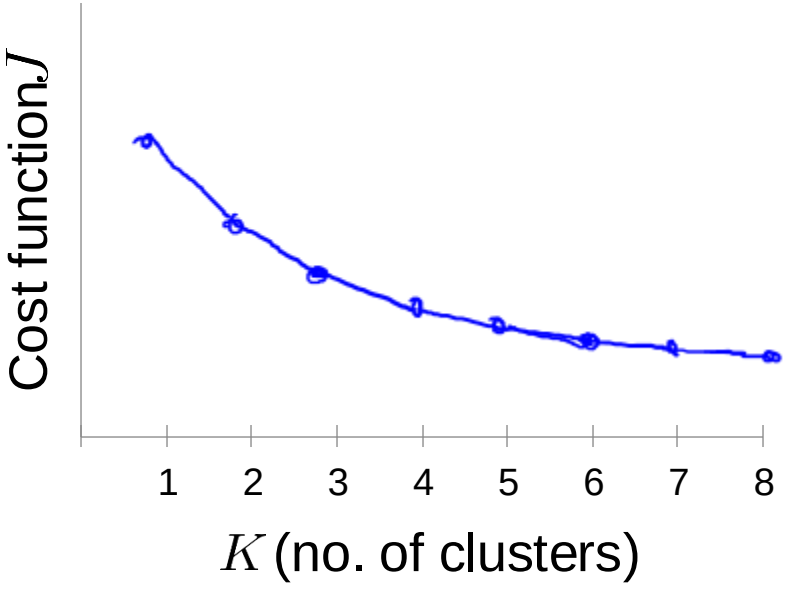
For i = 1 to 100 {

Randomly initialize K-means.
Run K-means. Get $c^{(1)}, \ldots, c^{(m)}, \mu_1, \ldots, \mu_K$.
Compute cost function (distortion)
$J(c^{(1)}, \ldots, c^{(m)}, \mu_1, \ldots, \mu_K)$
}

Pick clustering that gave lowest cost $J(c^{(1)}, \ldots, c^{(m)}, \mu_1, \ldots, \mu_K)$

选择合适聚类簇数K（Elbow方法）





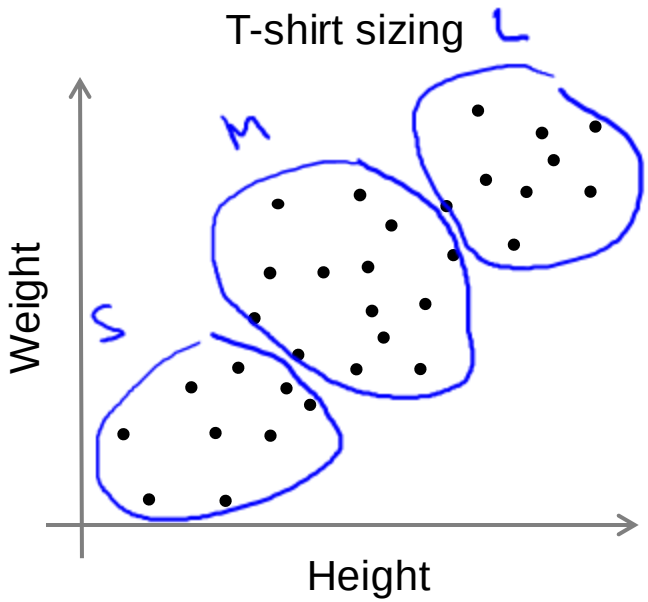
选择合适聚类簇数K

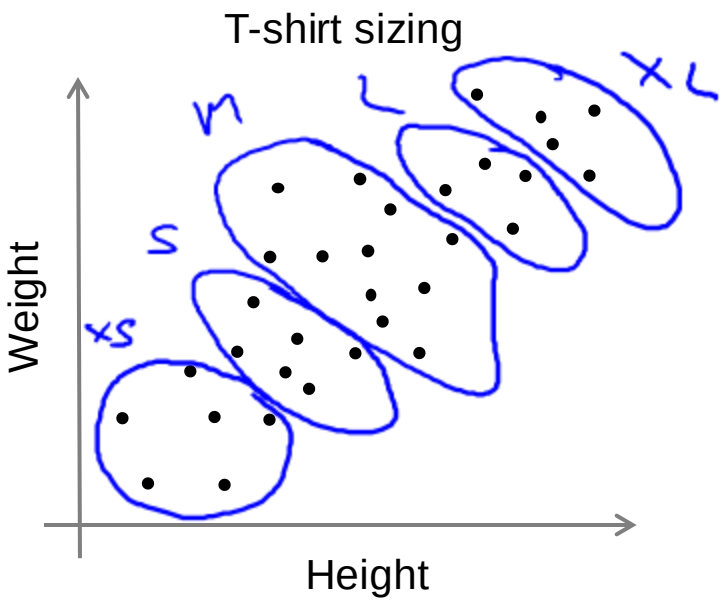
Sometimes, you’re running K-means to get clusters to use for some later/downstream purpose. Evaluate K-means based on a metric for how well it performs for that later purpose.

K=3 S, M, L

K=5 XS, S, M, L, XL

E.g.





4.2 Gaussian Mixture Model

输入: 样本集 $D = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_m\}$;
高斯混合成分个数 k.

过程:

初始化高斯混合分布的模型参数 $\{(\alpha_i, \boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i) \mid 1 \leqslant i \leqslant k\}$
repeat
  for $j = 1, 2, \ldots, m$ **do**
    根据式(9.30)计算 $\boldsymbol{x}_j$ 由各混合成分生成的后验概率, 即
    $\gamma_{ji} = p_{\mathcal{M}}(z_j = i \mid \boldsymbol{x}_j)$ $(1 \leqslant i \leqslant k)$
  end for

for $i = 1, 2, \ldots, k$ **do**

  计算新均值向量: $\boldsymbol{\mu}_i' = \frac{\sum_{j=1}^{m} \gamma_{ji} \boldsymbol{x}_j}{\sum_{j=1}^{m} \gamma_{ji}}$;

  计算新协方差矩阵: $\boldsymbol{\Sigma}_i' = \frac{\sum_{j=1}^{m} \gamma_{ji} (\boldsymbol{x}_j - \boldsymbol{\mu}_i')(\boldsymbol{x}_j - \boldsymbol{\mu}_i')^{\mathrm{T}}}{\sum_{j=1}^{m} \gamma_{ji}}$;

  计算新混合系数: $\alpha_i' = \frac{\sum_{j=1}^{m} \gamma_{ji}}{m}$;

end for

将模型参数 $\{(\alpha_i, \boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i) \mid 1 \leqslant i \leqslant k\}$ 更新为 $\{(\alpha_i', \boldsymbol{\mu}_i', \boldsymbol{\Sigma}_i') \mid 1 \leqslant i \leqslant k\}$

until 满足停止条件

$C_i = \varnothing \ (1 \leqslant i \leqslant k)$

for $j = 1, 2, \ldots, m$ **do**

  根据式(9.31)确定 $\boldsymbol{x}_j$ 的簇标记 λ_j;

  将 $\boldsymbol{x}_j$ 划入相应的簇: $C_{\lambda_j} = C_{\lambda_j} \bigcup \{\boldsymbol{x}_j\}$

end for

输出: 簇划分 $\mathcal{C} = \{C_1, C_2, \ldots, C_k\}$

- DBSCAN(Density-Based Spatial Clustering of Applications with Noise) 连通簇簇定义(P212)

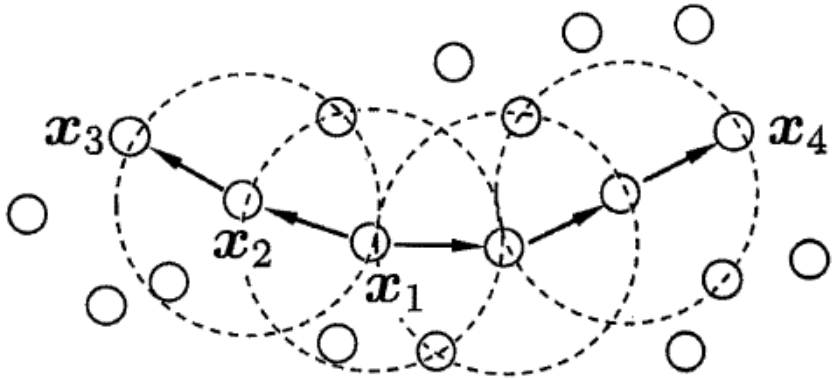


图 9.8 DBSCAN 定义的基本概念($MinPts = 3$): 虚线显示出 ϵ-邻域, x_1 是核心对象, x_2 由 x_1 密度直达, x_3 由 x_1 密度可达, x_3 与 x_4 密度相连.

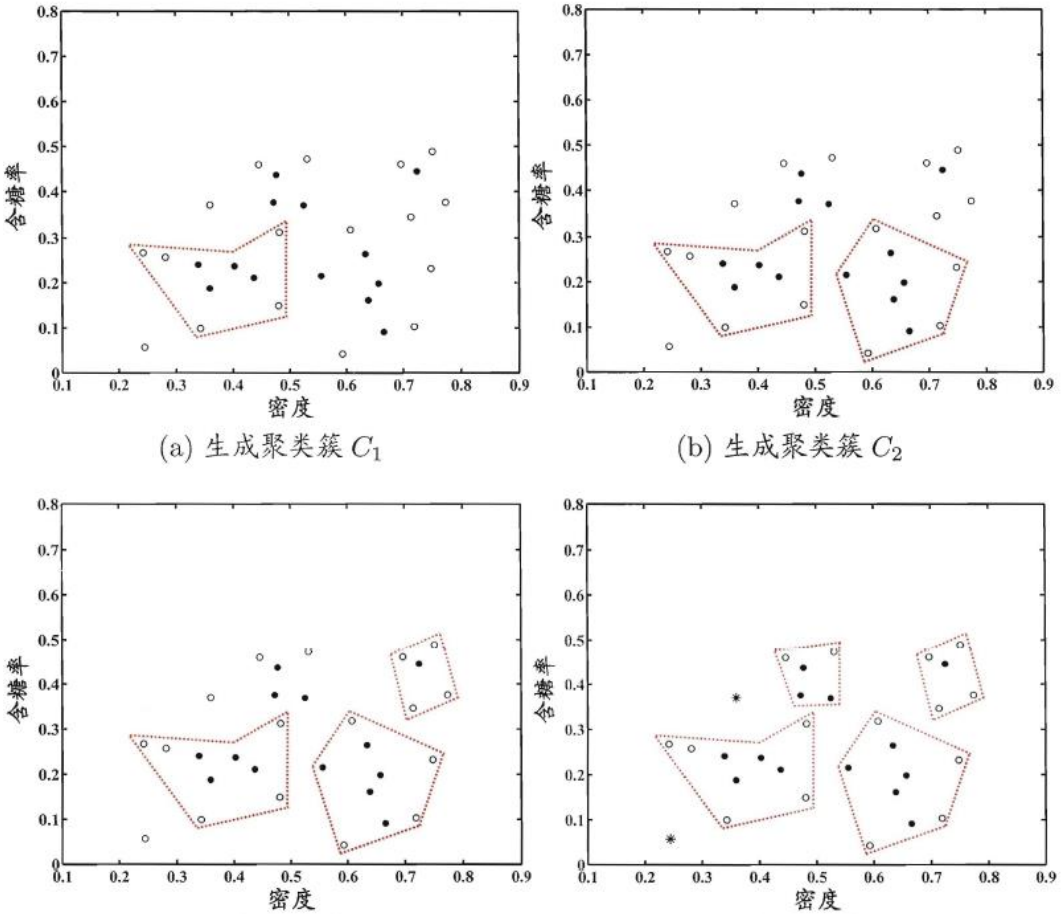
5. DBSCAN

输入: 样本集 $D = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_m\}$;
邻域参数 $(\epsilon, MinPts)$.

过程:

```
初始化核心对象集合: Ω = ∅
for j = 1, 2, ..., m do
    确定样本 x_j 的 ε-邻域 N_ε(x_j);
    if |N_ε(x_j)| ⩾ MinPts then
        将样本 x_j 加入核心对象集合: Ω = Ω ⋃ {x_j}
    end if
end for
```

```
初始化聚类簇数: k = 0
初始化未访问样本集合: Γ = D
while Ω ≠ ∅ do
    记录当前未访问样本集合: Γ_old = Γ;
    随机选取一个核心对象 o ∈ Ω, 初始化队列 Q =< o >;
    Γ = Γ \ {o};
    while Q ≠ ∅ do
        取出队列 Q 中的首个样本 q;
        if |N_ε(q)| ⩾ MinPts then
            令 Δ = N_ε(q) ⋂ Γ;
            将 Δ 中的样本加入队列 Q;
            Γ = Γ \ Δ;
        end if
    end while
    k = k + 1, 生成聚类簇 C_k = Γ_old \ Γ;
    Ω = Ω \ C_k
end while
```



(a) 生成聚类簇 C_1　(b) 生成聚类簇 C_2

(c) 生成聚类簇 C_3　(d) 生成聚类簇 C_4

图 9.10 DBSCAN 算法($\epsilon = 0.11$, $MinPts = 5$)生成聚类簇的先后情况. 核心对象、非核心对象、噪声样本分别用"•" "○" "*"表示, 红色虚线显示出簇划分.

6. Hierarchical Clustering

- 在不同层次对数据集进行划分，从而形成树形的聚类结构
  - “自底向上”的聚合策略 (AGNES)
  - “自顶向下”的分拆策略
- AGNES (Agglomerative Nesting, 凝聚聚类)

6. AGNES

输入: 样本集 $D = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_m\}$;
聚类簇距离度量函数 d;
聚类簇数 k.

过程:

for $j = 1, 2, \ldots, m$ **do**
  $C_j = \{\boldsymbol{x}_j\}$
end for
for $i = 1, 2, \ldots, m$ **do**
  for $j = 1, 2, \ldots, m$ **do**
    $M(i, j) = d(C_i, C_j)$;
    $M(j, i) = M(i, j)$
  end for
end for
设置当前聚类簇个数: $q = m$
while $q > k$ **do**
  找出距离最近的两个聚类簇 C_{i^*} 和 C_{j^*};
  合并 C_{i^*} 和 C_{j^*}: $C_{i^*} = C_{i^*} \bigcup C_{j^*}$;
  for $j = j^* + 1, j^* + 2, \ldots, q$ **do**
    将聚类簇 C_j 重编号为 C_{j-1}
  end for
  删除距离矩阵 M 的第 j^* 行与第 j^* 列;
  for $j = 1, 2, \ldots, q - 1$ **do**
    $M(i^*, j) = d(C_{i^*}, C_j)$;
    $M(j, i^*) = M(i^*, j)$
  end for
  $q = q - 1$
end while

输出: 簇划分 $\mathcal{C} = \{C_1, C_2, \ldots, C_k\}$

6. AGNES

- 类-类距离

$$\text{最小距离: } d_{\min}(C_i, C_j) = \min_{\boldsymbol{x} \in C_i, \boldsymbol{z} \in C_j} \operatorname{dist}(\boldsymbol{x}, \boldsymbol{z}) \ , \tag{9.41}$$

$$\text{最大距离: } d_{\max}(C_i, C_j) = \max_{\boldsymbol{x} \in C_i, \boldsymbol{z} \in C_j} \operatorname{dist}(\boldsymbol{x}, \boldsymbol{z}) \ , \tag{9.42}$$

$$\text{平均距离: } d_{\text{avg}}(C_i, C_j) = \frac{1}{|C_i||C_j|} \sum_{\boldsymbol{x} \in C_i} \sum_{\boldsymbol{z} \in C_j} \operatorname{dist}(\boldsymbol{x}, \boldsymbol{z}) \ . \tag{9.43}$$

- 对象-类距离

- 对象-对象距离

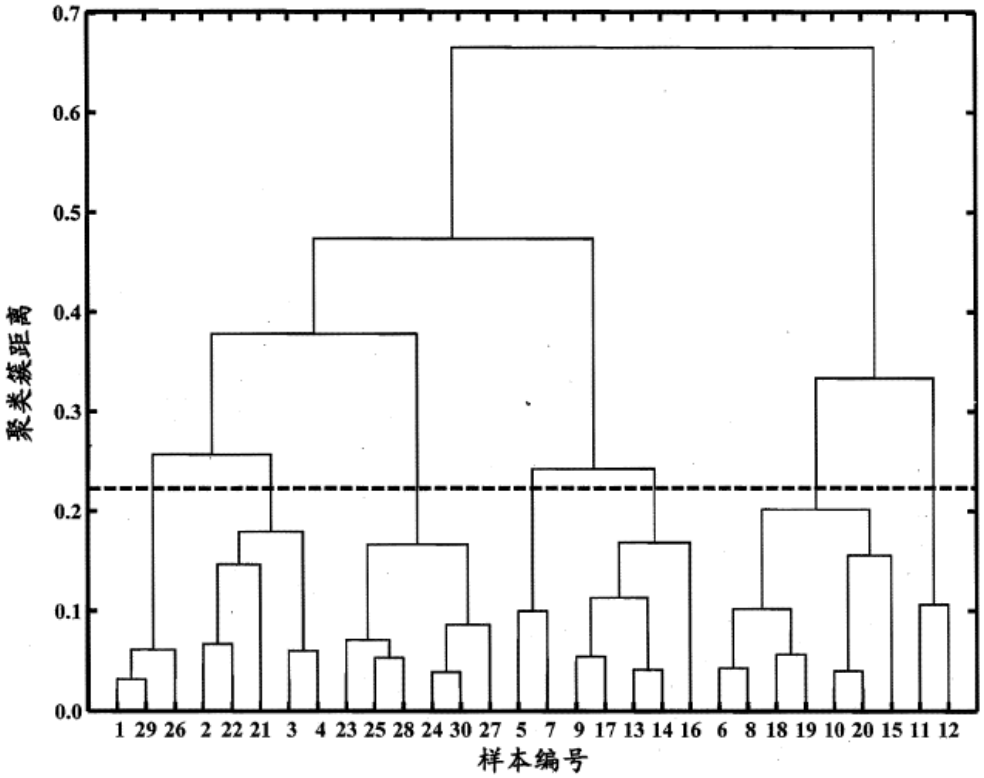
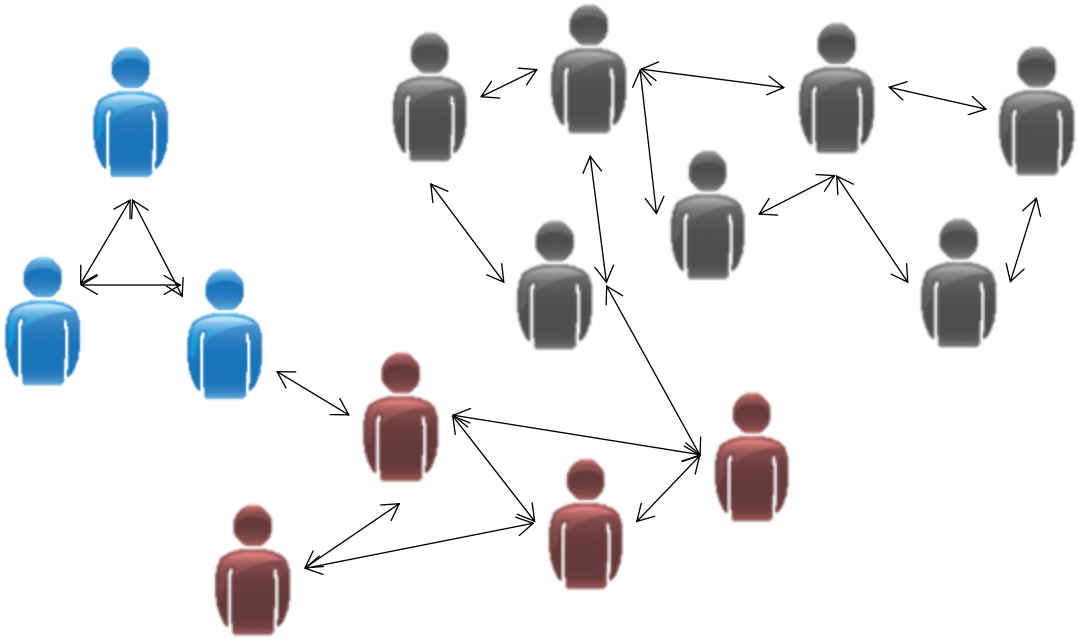


图 9.12 西瓜数据集 4.0 上 AGNES 算法生成的树状图(采用 $d_{\max}$). 横轴对应于样本编号, 纵轴对应于聚类簇距离.

其他：网络数据聚类算-Mincut



7. 双向层次聚类结果的可视化

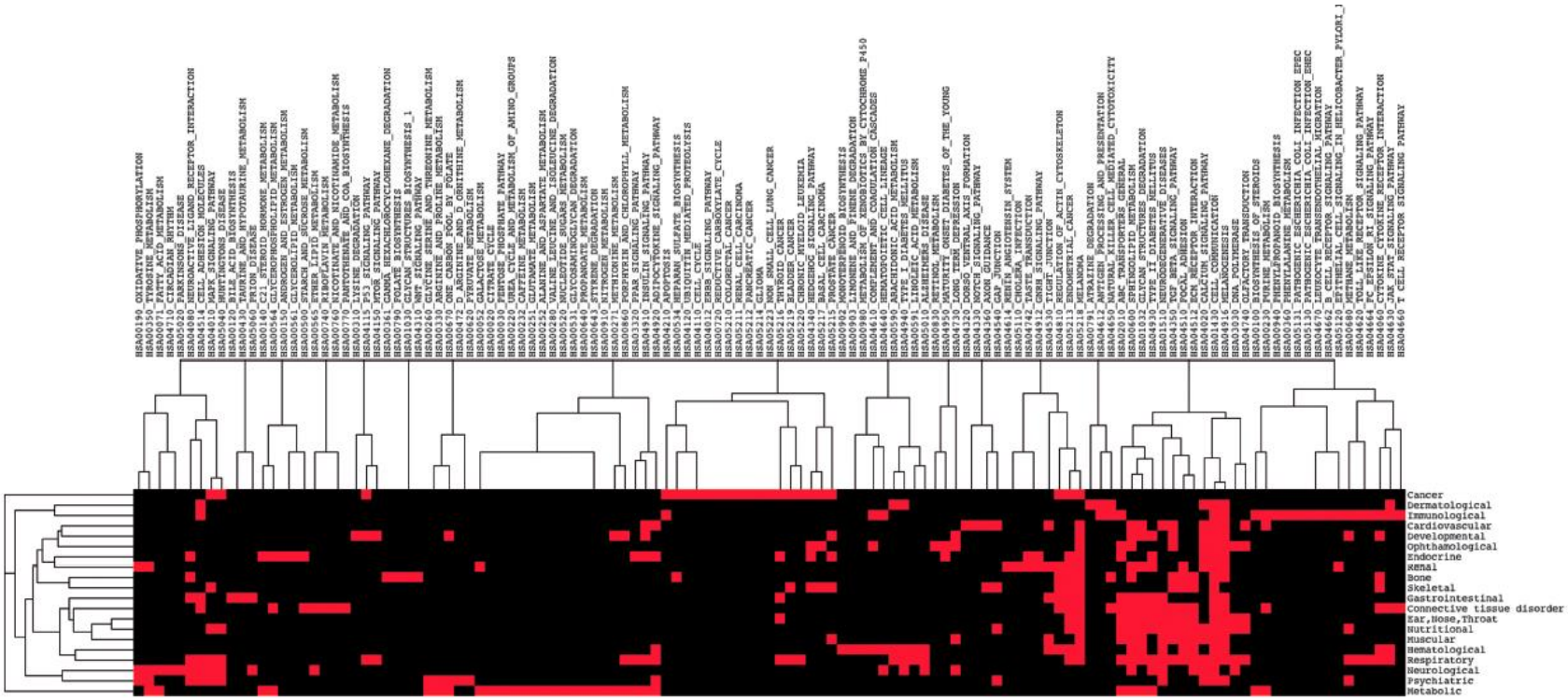
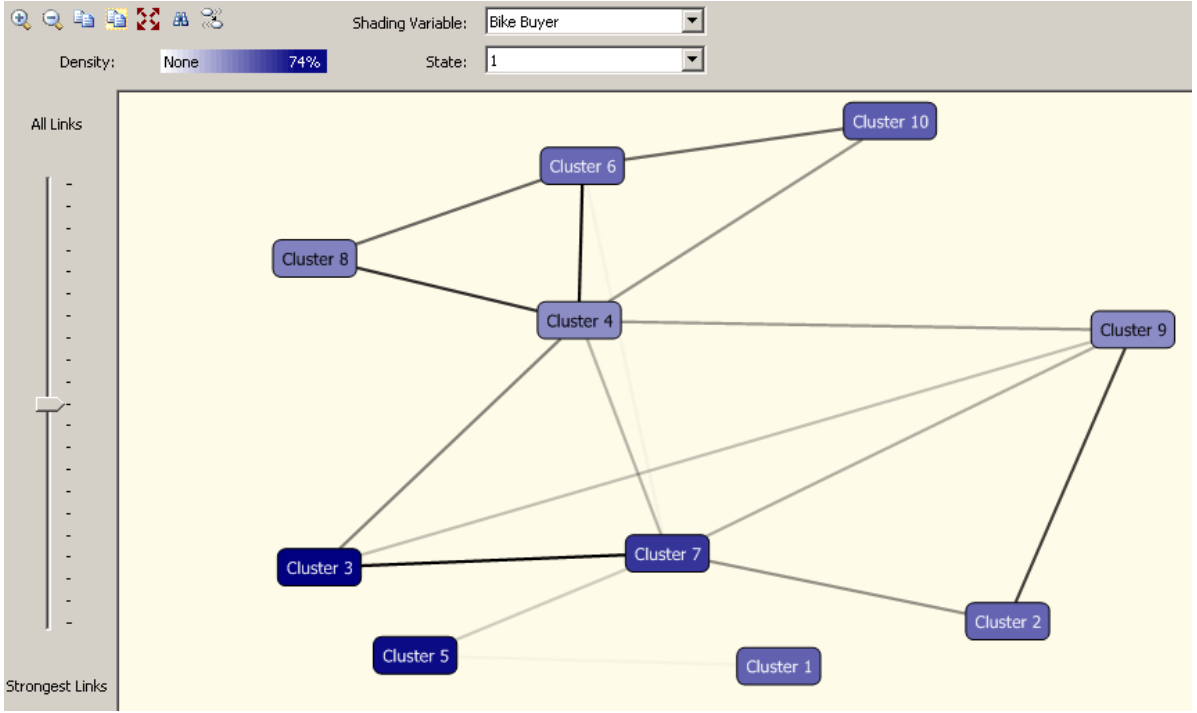


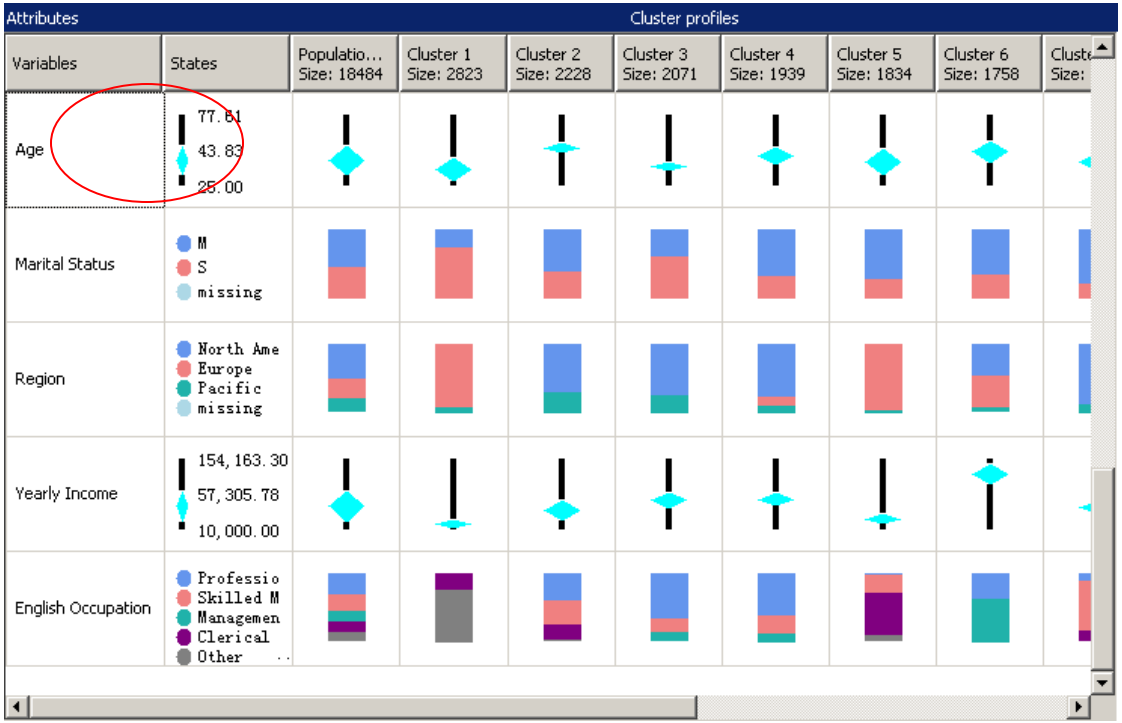
Figure 6. Predicted associations between disease classes and pathways. Each red entry represents a predicted association between 20 disease classes and 200 KEGG pathways.

7. 聚类结果可视化



- The lines between the clusters represent “closeness”
- The color of the cluster represents the frequency of the variable and state

其他：聚类结果可视化



- The distribution of an attribute's states for each cluster
- A colored bar: discrete attribute
- A diamond chart: continuous attribute

7. 聚簇特征

Characteristics for Cluster 3

Variables	Values	Probability
Bike Buyer	1	
Number Children At Home	0	
Region	North America	
Age	36.2 - 43.8	
English Occupation	Professional	
Marital Status	S	
House Owner Flag	1	
Gender	F	
First Name	missing	
English Education	Bachelors	
Commute Distance	0-1 Miles	
Yearly Income	57305.8 - 79082.2	
Number Cars Owned	0	
Gender	M	
Number Cars Owned	1	
English Education	Graduate Degree	
House Owner Flag	0	
Last Name	missing	
Marital Status	M	
Commute Distance	2-5 Miles	
Total Children	0	
Region	Pacific	

- The characteristics that make up a cluster in more detail

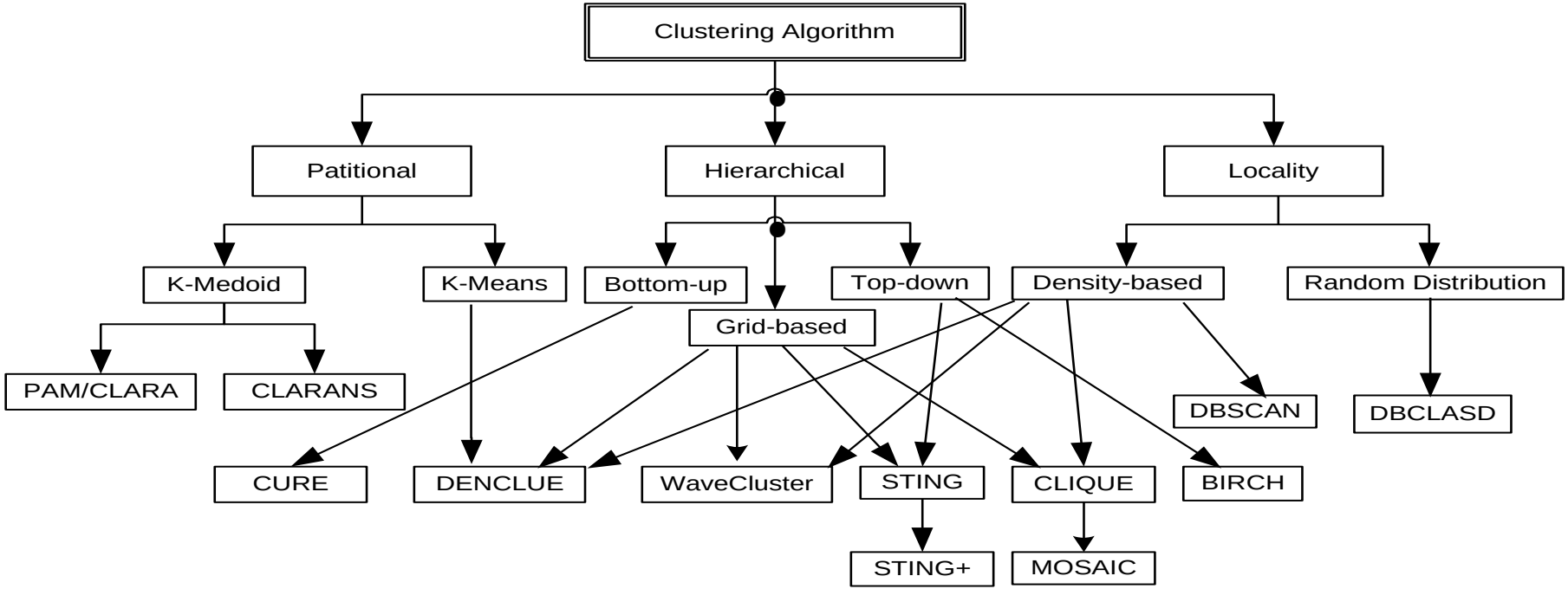
7. 区分簇的典型特征

Discrimination scores for Cluster 3 and Cluster 4

Variables	Values	Favors Cluster 3	Favors Cluster 4
Number Children At Home	0		
Age	27.9 - 43.5		
Age	43.5 - 95.0		
Total Children	0		
English Education	Graduate Degree		
Commute Distance	10+ Miles		
English Education	Partial College		
Bike Buyer	0		
Bike Buyer	1		
Total Children	4		
Number Cars Owned	2		
Number Cars Owned	3		
Number Children At Home	1		
Commute Distance	0-1 Miles		
Total Children	5		
Total Children	1		
English Education	High School		
Number Cars Owned	0		
Number Children At Home	4		
House Owner Flag	1		
House Owner Flag	0		
Number Children At Home	3		

- The characteristics that distinguish one cluster from another

常见的聚类算法之间的关系



其他的聚类(Clustering)注意事项

- 可伸缩性
- 可以处理噪声
- 对输入次序不敏感
- 能够处理高维数据
- 可解释和可用性
- 处理不同类型属性的能力
- 可以发现任意形状的簇
- 用于决定输入参数的领域知识最小化

总结

1. 聚类简介
2. 聚类性能评价指标
3. 空间和距离（相似度）度量
4. 基于划分的聚类 (K-Means, GMM)
5. 基于密度的聚类 (DBSCAN)
6. 层次聚类方法 (AGNES)
7. 聚类可视化