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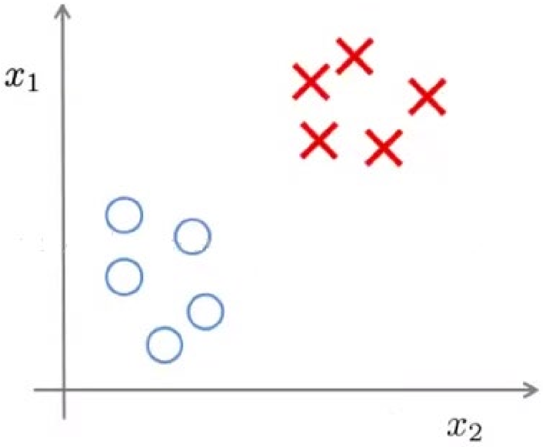
Chapter 11 Clustering

Outline

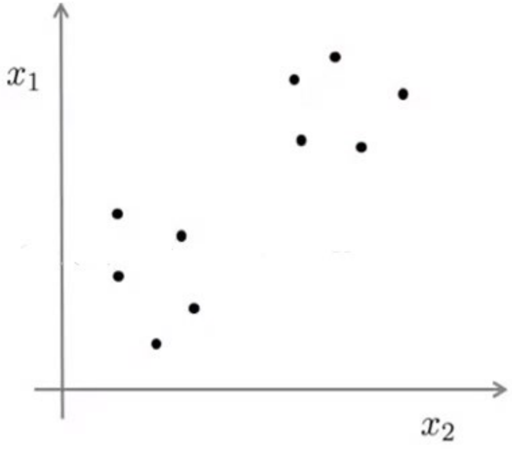
- Definition
- Distance Calculation
- Algorithms
  - K-means
  - Mixture of Gaussian
  - DBSCAN
  - AGNES
- Performance Measure

Definition

- Supervised learning VS. Unsupervised learning
- In supervised learning, we know something(label or value) about data(X={x1,…,xn}, Y={y1,…,yn}known), learn y = f (x)
- In unsupervised learning, we know nothing about the data(X known, Y unknown).



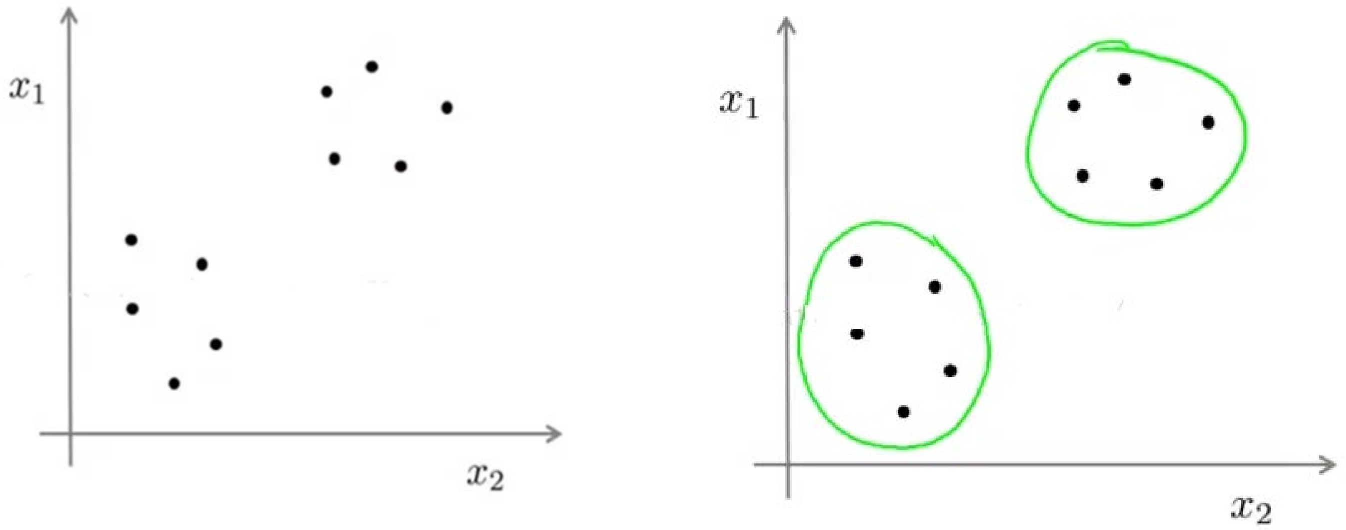
Supervised Learning



Unsupervised Learning

Definition

- Clustering is the task of grouping a set of objects in such a way that objects in the same group(intra-group) are more similar to each other than to those in other groups(inter-group) .



Distance Calculation

- Minkowski distance

$$dist_{mk}(x_i\,,x_j) = (\sum_{u=1}^{n} |x_{iu} - x_{ju}|^p)^{\frac{1}{p}}$$

$$x_i = (x_{i1}; x_{i2}; \ldots x_{in}), x_j = (x_{j1}\ x_{j2}; \ldots x_{jn})$$

- Euclidean distance (p=2)
- Manhattan distance (p=1)

$$x_1=[2,1] \qquad \xrightarrow{\textbf{Manhattan distance}} \qquad d=(|2-3|^1+|1-3|^1)^1=3$$

$$x_2=[3,3] \qquad \xrightarrow{\textbf{Euclidean distance}} \qquad d=(|2-3|^2+|1-3|^2)^{1/2}=\sqrt{5}$$

Other Similarity Metrics

- Chebyshev Distance D=max($|x_1 - x_2|$,$|y_1 - y_2|$)
- Cosine

$$\cos(\theta) = \frac{\sum_{i=1}^{n}(x_i * y_i)}{\sqrt{\sum_{i=1}^{n}(x_i)^2} * \sqrt{\sum_{i=1}^{n}(y_i)^2}}$$

- Hamming Distance d(x,y)=$\sum X[i] \oplus Y[i]$
- Jaccard Distance

$$\frac{|A \cup B| - |A \cap B|}{|A \cup B|}$$

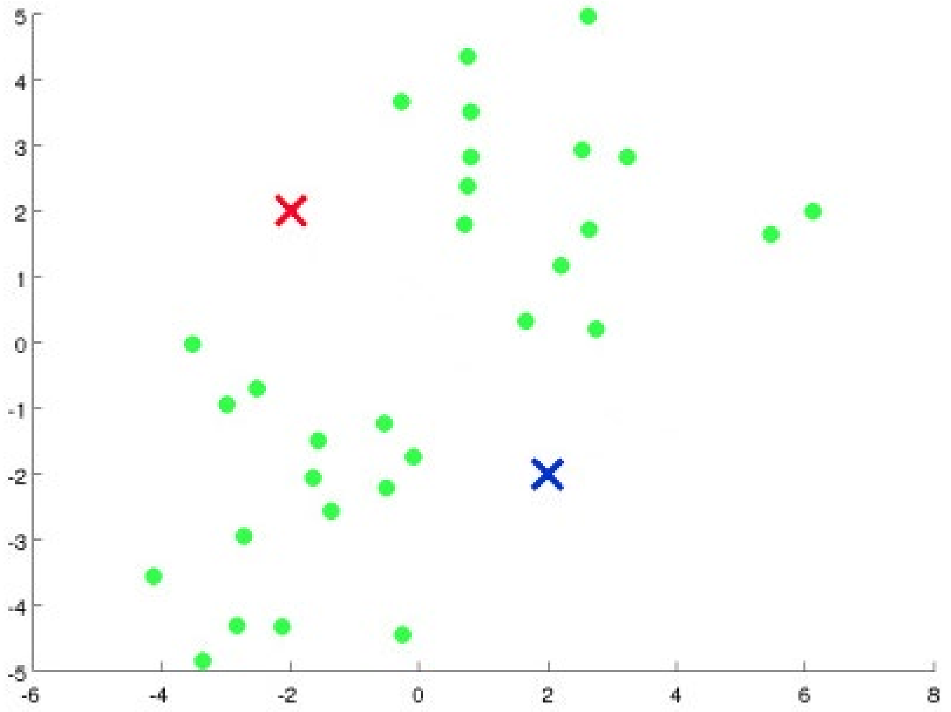
- Correlation coefficient and Correlation distance

Algorithm--K-means

- Randomly select K samples as the centroids of clustering.
- Calculate the distances of each sample from the K centroid points.
- Select the cluster centroid $c_i\ (i = 1,2 \ldots K)$with the smallest distance to divide the cluster.
- Re-determine the centroids.
- Iterate until it converges.

K-means

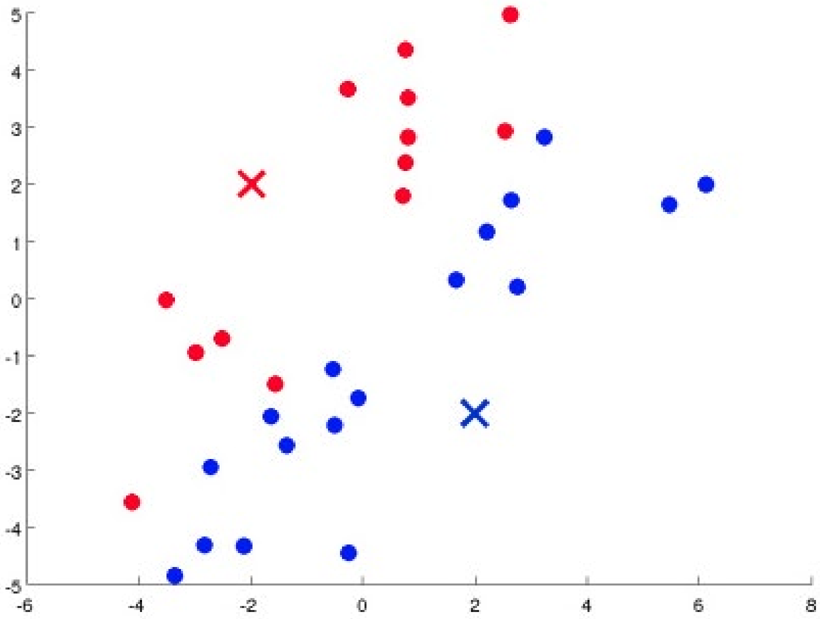
- By experience, set k=2 .
- Randomly select two points as cluster centroids.



K-means

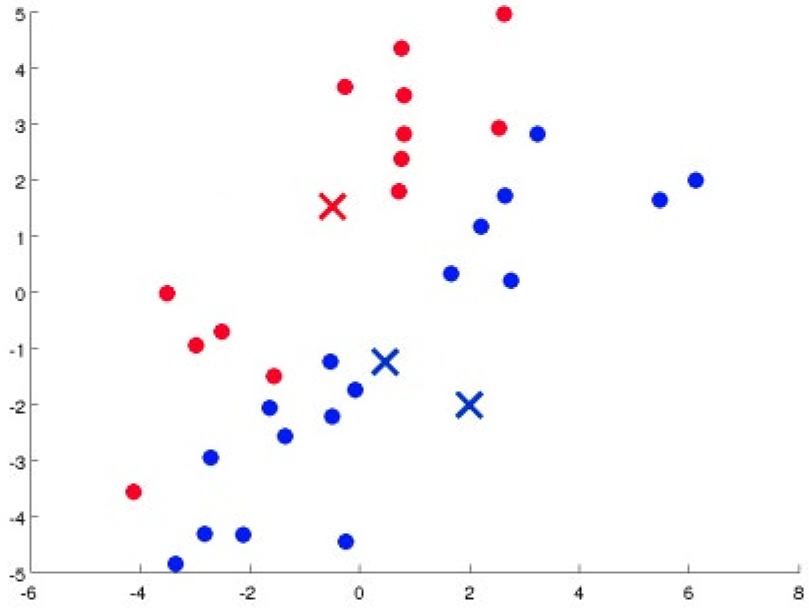
- For all green samples, compute distances from the blue point and red point.
- Choose the smallest distance and assign it to one cluster.

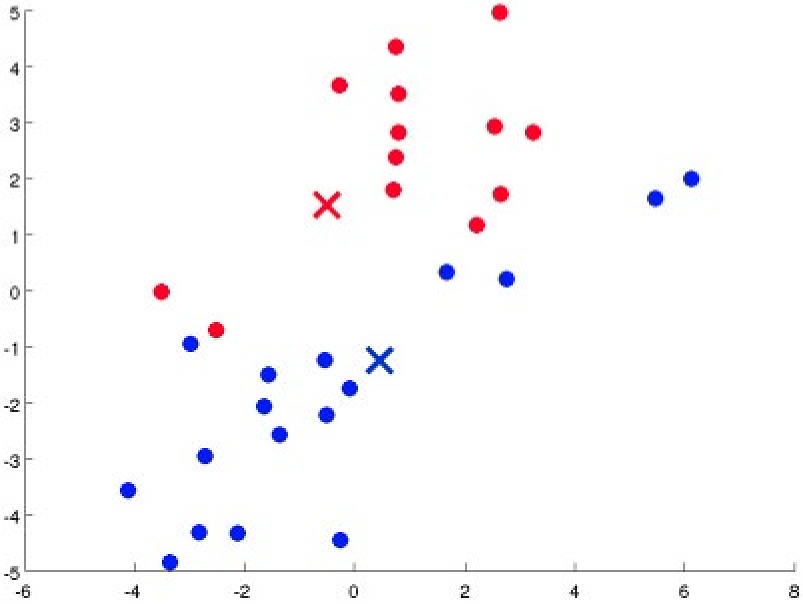
簇划分



K-means

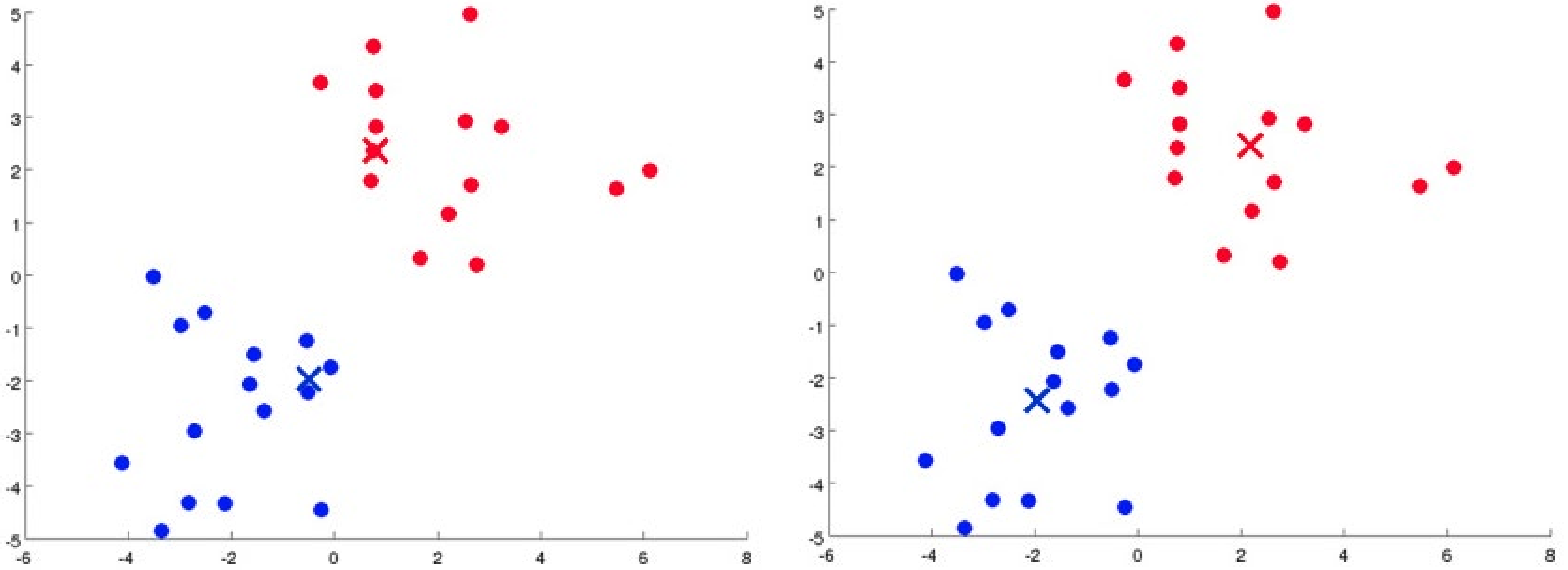
- Compute the average for two clusters.
- Re-determine cluster centroids.



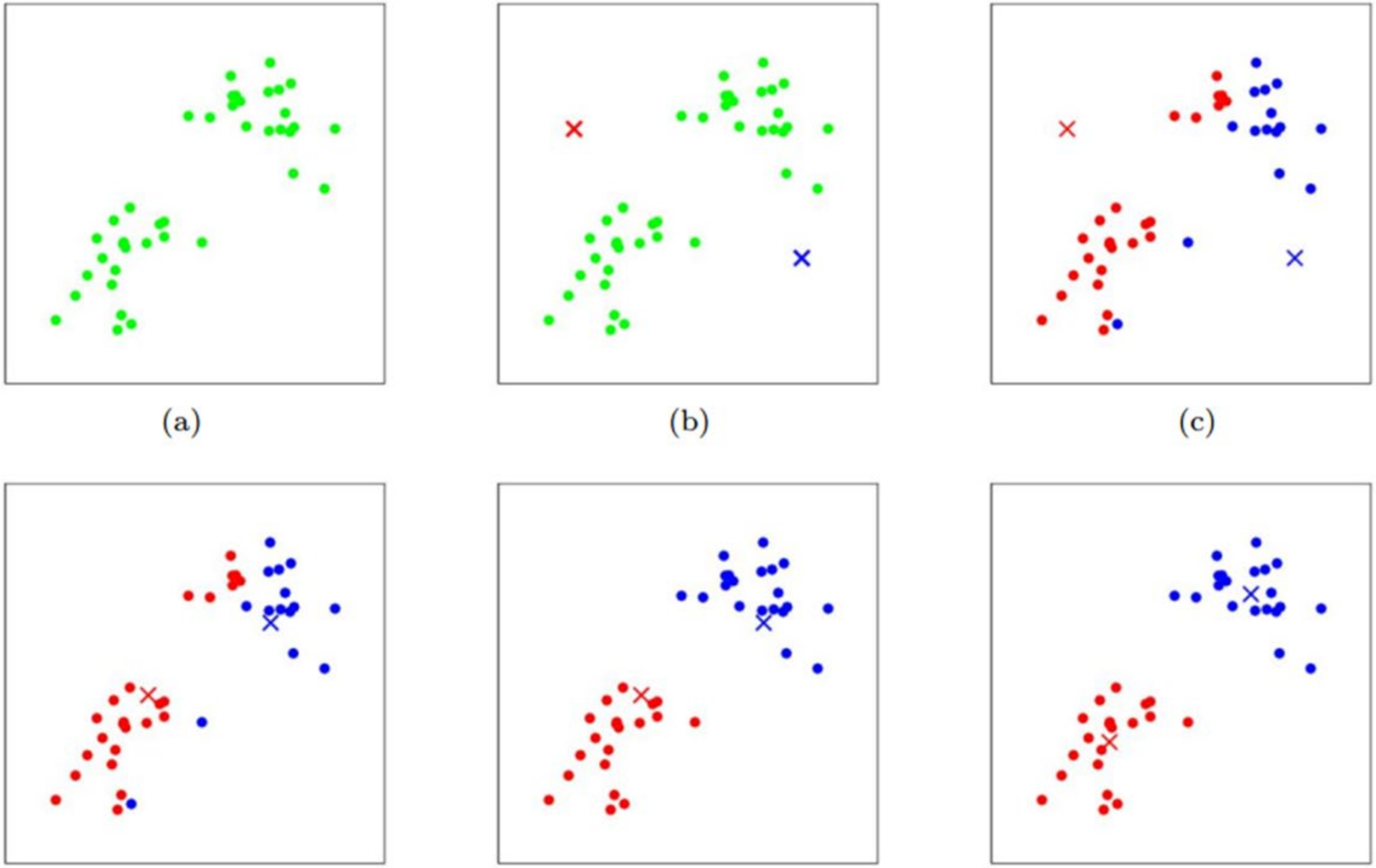


K-means

- Iterate until convergence (the cluster centroids will not change).



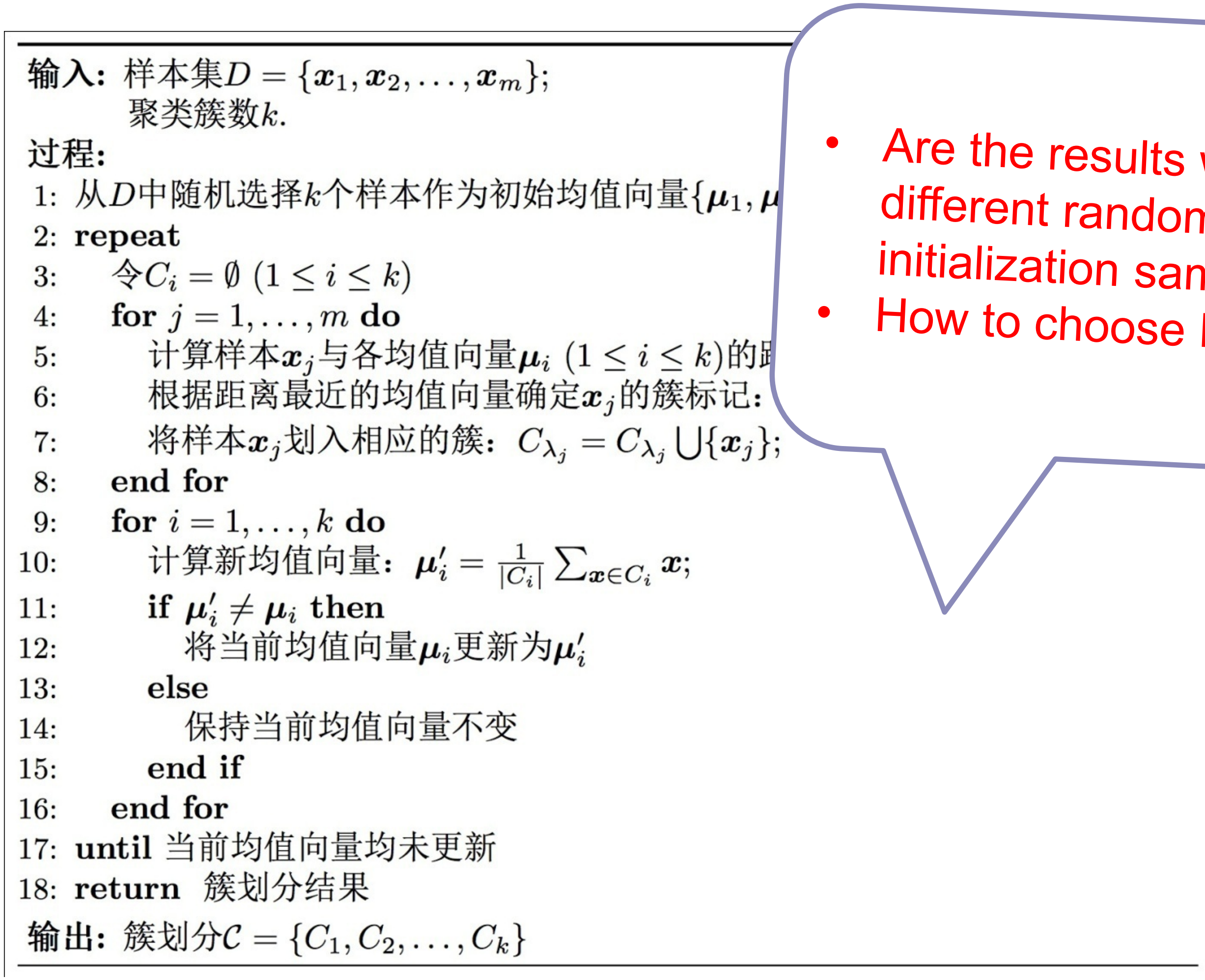
K-means



(a) (b) (c)

(d) (e) (f)

K-means



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输入：样本集$D = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_m\}$;
      聚类簇数$k$.
过程：
从$D$中随机选择$k$个样本作为初始均值向量$\{\boldsymbol{\mu}_1, \boldsymbol{\mu}$
repeat
    令$C_i = \emptyset \; (1 \leq i \leq k)$
    for $j = 1, \ldots, m$ do
        计算样本$\boldsymbol{x}_j$与各均值向量$\boldsymbol{\mu}_i \; (1 \leq i \leq k)$的距
        根据距离最近的均值向量确定$\boldsymbol{x}_j$的簇标记：
        将样本$\boldsymbol{x}_j$划入相应的簇：$C_{\lambda_j} = C_{\lambda_j} \bigcup \{\boldsymbol{x}_j\}$;
    end for
    for $i = 1, \ldots, k$ do
        计算新均值向量：$\boldsymbol{\mu}'_i = \frac{1}{|C_i|} \sum_{\boldsymbol{x} \in C_i} \boldsymbol{x}$;
        if $\boldsymbol{\mu}'_i \neq \boldsymbol{\mu}_i$ then
            将当前均值向量$\boldsymbol{\mu}_i$更新为$\boldsymbol{\mu}'_i$
        else
            保持当前均值向量不变
        end if
    end for
until 当前均值向量均未更新
return 簇划分结果
输出：簇划分$\mathcal{C} = \{C_1, C_2, \ldots, C_k\}$
```

簇划分

移动
聚类中心

- Are the results with different random initialization same?
- How to choose K?

K-means

- We need all possible initializations and get the best result.
- The measure to find the best result is minimizing square error E(SSE, sum of the Squared Error).

$$\mathrm{E} = \sum_{i=1}^{k} \sum_{x \in C_i} \|x - u_i\|_2^2 \qquad \mathrm{E} = \sum_{i=1}^{m} \left\|x_i - u_{\lambda_i}\right\|_2^2$$

$$u_i = \frac{1}{|C_i|} \sum_{x \in C_i} x$$

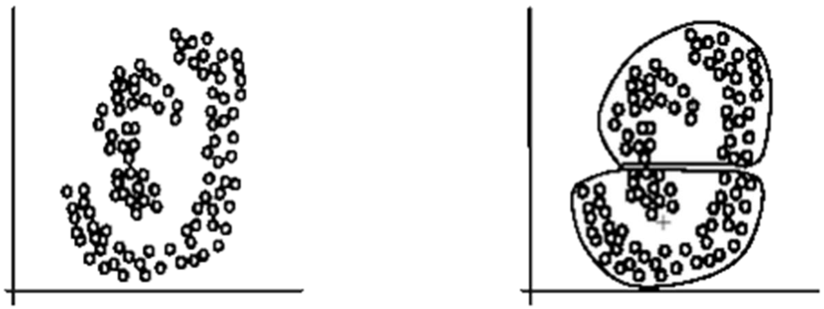
K-means

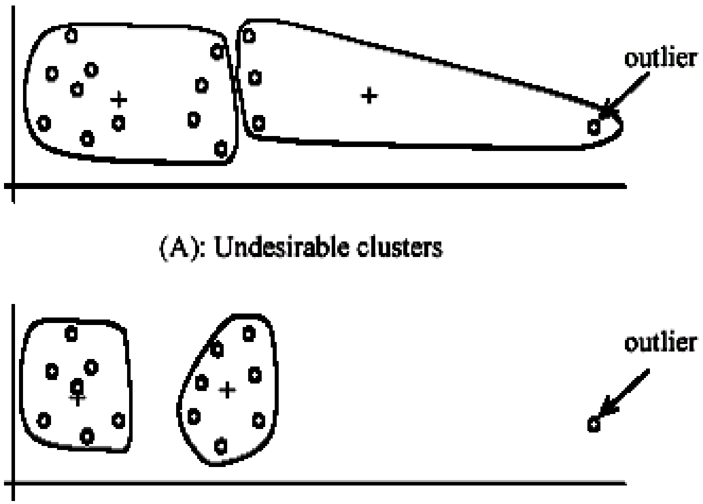
How to initialize

- It is NP-Hard to minimizing E.
- K-means uses an iterative optimal algorithm. Each step of every iteration is the process of optimizing E.
- We can choose multiple initializations to get the best result(Attention: Whether this measure is effective depends on k).

K-means

- K-means is not always suitable.





(A): Undesirable clusters

(B): Ideal clusters

Mixture of Gaussian

- Gaussian mixture distribution

$$p(x) = \sum_{k=1}^{K} p(k)p(x|k)$$
$$= \sum_{k=1}^{K} \pi_k \mathcal{N}(x|\mu_k, \Sigma_k)$$

- $\boldsymbol{\mu_i}$, $\boldsymbol{\Sigma_i}$: mean vector and covariance matrix of i_{th} mixed component
- $\boldsymbol{\pi_k}$: corresponding mixture coefficient

Mixture of Gaussian

- Objective function：

$$\sum_{i=1}^{N} \log\left\{\sum_{k=1}^{K} \pi_k \mathcal{N}(x_i|\mu_k, \Sigma_k)\right\}$$

- Then， we use MLE(Maximum likelihood estimate) to optimize function.

Mixture of Gaussian

- 估计数据由每个 Component 生成的概率（并不是每个 Component 被选中的概率）：对于每个数据 x_i 来说，它由第 k 个 Component 生成的概率为

$$\gamma(i,k) = \frac{\pi_k \mathcal{N}(x_i|\mu_k,\Sigma_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(x_i|\mu_j,\Sigma_j)}$$

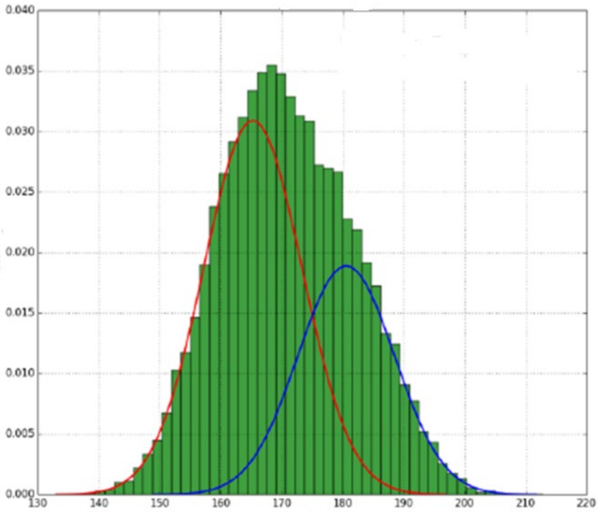
- 估计每个 Component 的参数

$$\mu_k = \frac{1}{N_k}\sum_{i=1}^{N}\gamma(i,k)x_i$$

$$\Sigma_k = \frac{1}{N_k}\sum_{i=1}^{N}\gamma(i,k)(x_i-\mu_k)(x_i-\mu_k)^T$$

Mixture of Gaussian

- Suppose we have 100 students and the only data we can get is their height. Try to model the distribution of male and female.
- The height obeys Gaussian distribution.

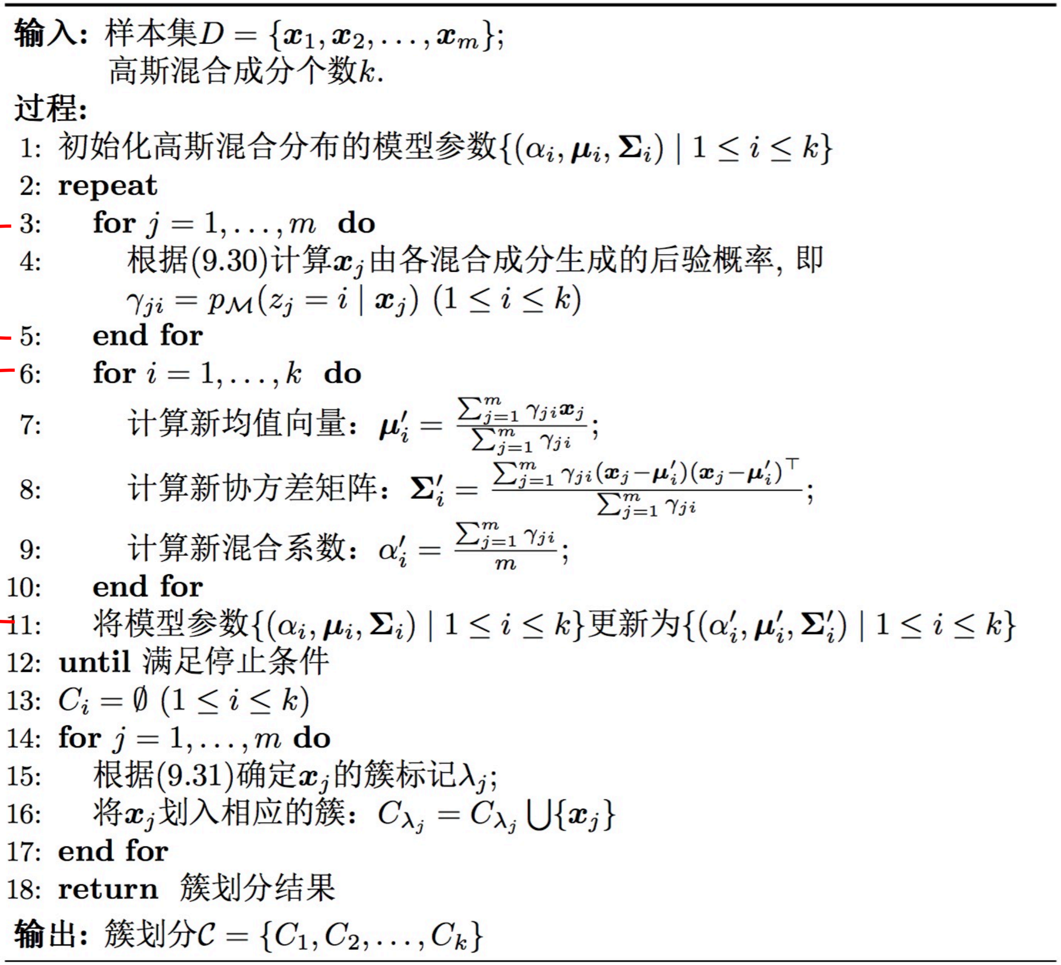


Mixture of Gaussian

先假定男生服从参数为~N(180,10)的高斯分布，女生服从参数为~N(160,8)的高斯分布(Assume a determined Gaussian model for boys and girls)

- 对每个样本计算出分别属于男生和女生的概率(Compute the probability that clustering each sample to boys and girls)
- 认定：每个样本分属于男生和女生的部分（即概率，用$\gamma(i,k)$表示，即第i个样本属于第k个类别的概率）同样服从高斯分布，且具有更好的拟合属性。(如一个样本身高175，我们可以通过设定的参数计算出他有80%的概率为男生，20%的概率为女生，那可以把这个样本看作由80%的男生和20%的女生组成，并将这个样本看作是一个80%的男生样本和一个20%的女生样本。)(Divide each sample into two components according to the probability in step 2)
- 根据每个样本的男生组分和女生组分拟合出新的高斯模型。(Update the parameters according to the components in step 3)
- 迭代直到收敛。(Iterating these steps until convergence)

Mixture of Gaussian



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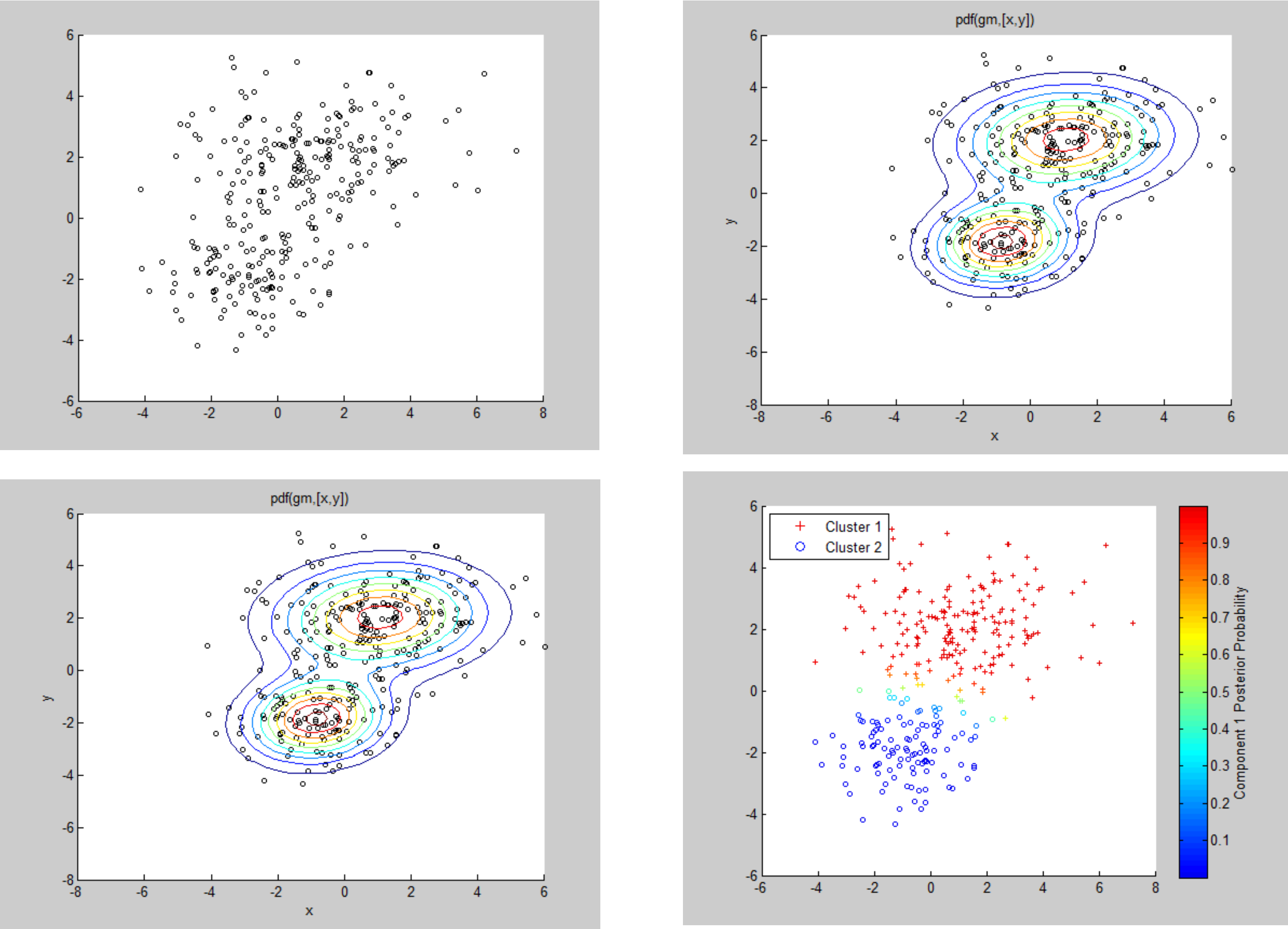
输入：样本集$D = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_m\}$;
      高斯混合成分个数$k$.
过程：
初始化高斯混合分布的模型参数$\{(\alpha_i, \boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i) \mid 1 \le i \le k\}$
repeat
    for $j = 1, \ldots, m$ do
        根据(9.30)计算$\boldsymbol{x}_j$由各混合成分生成的后验概率, 即
        $\gamma_{ji} = p_{\mathcal{M}}(z_j = i \mid \boldsymbol{x}_j)\ (1 \le i \le k)$
    end for
    for $i = 1, \ldots, k$ 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：$\boldsymbol{\Sigma}'_i = \frac{\sum_{j=1}^{m} \gamma_{ji} (\boldsymbol{x}_j - \boldsymbol{\mu}'_i)(\boldsymbol{x}_j - \boldsymbol{\mu}'_i)^{\top}}{\sum_{j=1}^{m} \gamma_{ji}}$;
        计算新混合系数：$\alpha'_i = \frac{\sum_{j=1}^{m} \gamma_{ji}}{m}$;
    end for
    将模型参数$\{(\alpha_i, \boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i) \mid 1 \le i \le k\}$更新为$\{(\alpha'_i, \boldsymbol{\mu}'_i, \boldsymbol{\Sigma}'_i) \mid 1 \le i \le k\}$
until 满足停止条件
$C_i = \emptyset\ (1 \le i \le k)$
for $j = 1, \ldots, m$ do
    根据(9.31)确定$\boldsymbol{x}_j$的簇标记$\lambda_j$;
    将$\boldsymbol{x}_j$划入相应的簇：$C_{\lambda_j} = C_{\lambda_j} \bigcup \{\boldsymbol{x}_j\}$
end for
return 簇划分结果
输出：簇划分$\mathcal{C} = \{C_1, C_2, \ldots, C_k\}$
```

固定模型参数
更新后验概率

固定后验概率
更新模型参数

Mixture of Gaussian

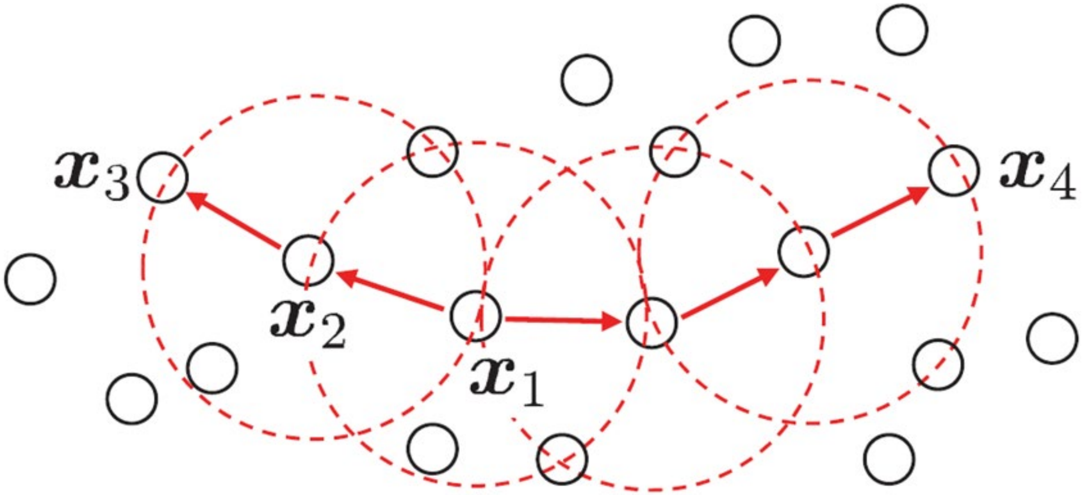


DBSCAN

- It is a famous density-based-clustering.
- ϵ-neighborhood:$N_{\epsilon}\left(x_j\right) = \{x_i \in D|dist(x_i, x_j\ ) \leq \epsilon)$ of the point x_j
- core object :a point with a $\left|N_{\epsilon}\left(x_j\right)\right| \geq MinPts$
- Directly density-reached: x_j is directly density-reachable from a core object x_i if x_j is in $N_{\epsilon}(x_i)$
- Density-reached: x_j is density-reachable from a core object x_i if a sequence of core objects $p_1, p_2,\ldots\ p_n$ between x_i and x_j exists and $p_{i+1}$is directly density-reached from p_i.
- Density-connected: x_i and x_j are density-connected if they are density-reachable from a common core object x_k.

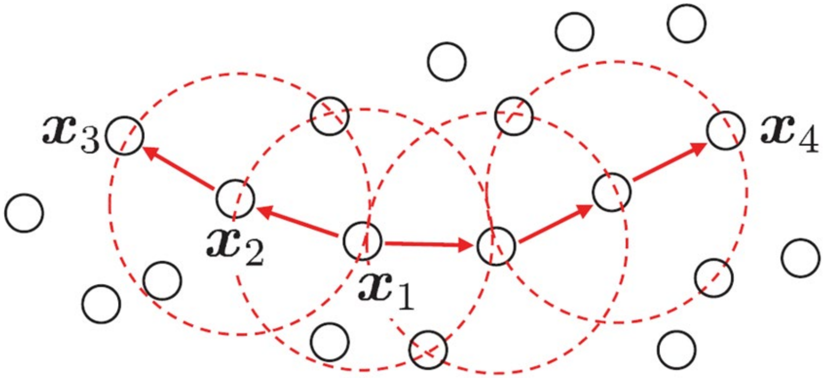
DBSCAN

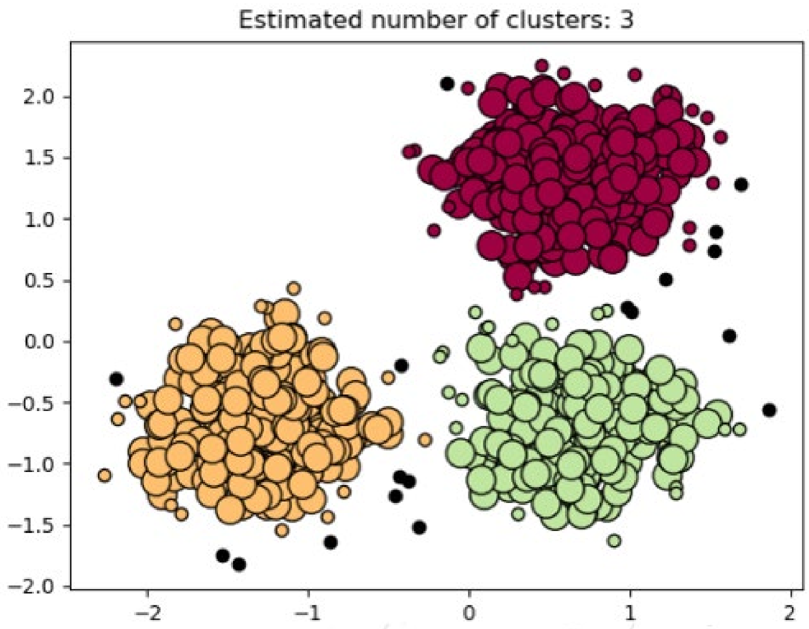
- Directly density-reached： X2 from X1
- Density-reached: X3 from X1
- Density-connected： X4 from X3



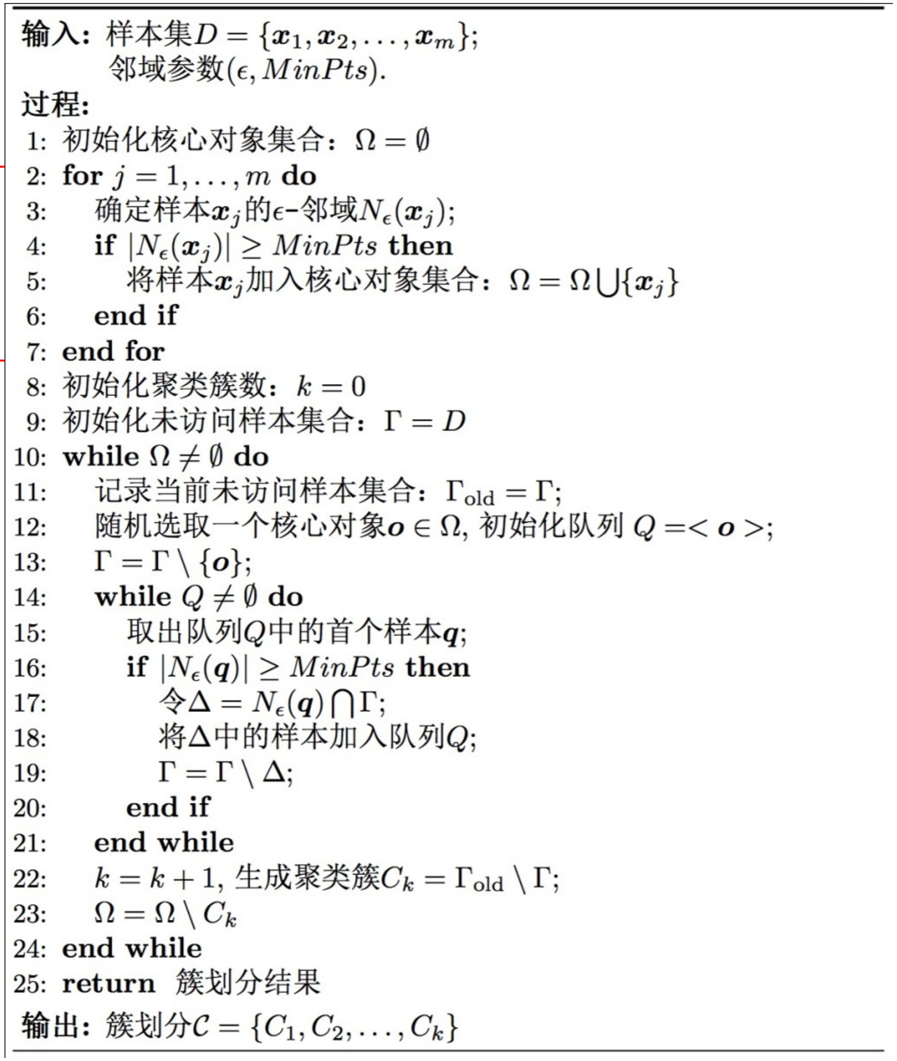
DBSCAN

- DBSCAN defines cluster as such sample set which is most density-connected.





DBSCAN



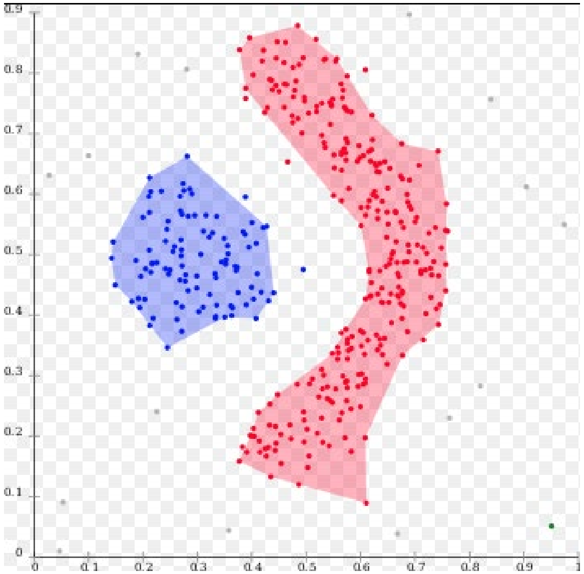
```
输入: 样本集$D = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_m\}$;
      邻域参数$(\epsilon, MinPts)$.
过程:
初始化核心对象集合: $\Omega = \emptyset$
for $j = 1, \ldots, m$ do
    确定样本$\boldsymbol{x}_j$的$\epsilon$-邻域$N_\epsilon(\boldsymbol{x}_j)$;
    if $|N_\epsilon(\boldsymbol{x}_j)| \geq MinPts$ then
        将样本$\boldsymbol{x}_j$加入核心对象集合: $\Omega = \Omega \bigcup \{\boldsymbol{x}_j\}$
    end if
end for
初始化聚类簇数: $k = 0$
初始化未访问样本集合: $\Gamma = D$
while $\Omega \neq \emptyset$ do
    记录当前未访问样本集合: $\Gamma_{\text{old}} = \Gamma$;
    随机选取一个核心对象$\boldsymbol{o} \in \Omega$, 初始化队列 $Q = < \boldsymbol{o} >$;
    $\Gamma = \Gamma \setminus \{\boldsymbol{o}\}$;
    while $Q \neq \emptyset$ do
        取出队列$Q$中的首个样本$\boldsymbol{q}$;
        if $|N_\epsilon(\boldsymbol{q})| \geq MinPts$ then
            令$\Delta = N_\epsilon(\boldsymbol{q}) \bigcap \Gamma$;
            将$\Delta$中的样本加入队列$Q$;
            $\Gamma = \Gamma \setminus \Delta$;
        end if
    end while
    $k = k + 1$, 生成聚类簇$C_k = \Gamma_{\text{old}} \setminus \Gamma$;
    $\Omega = \Omega \setminus C_k$
end while
return 簇划分结果
输出: 簇划分$\mathcal{C} = \{C_1, C_2, \ldots, C_k\}$
```

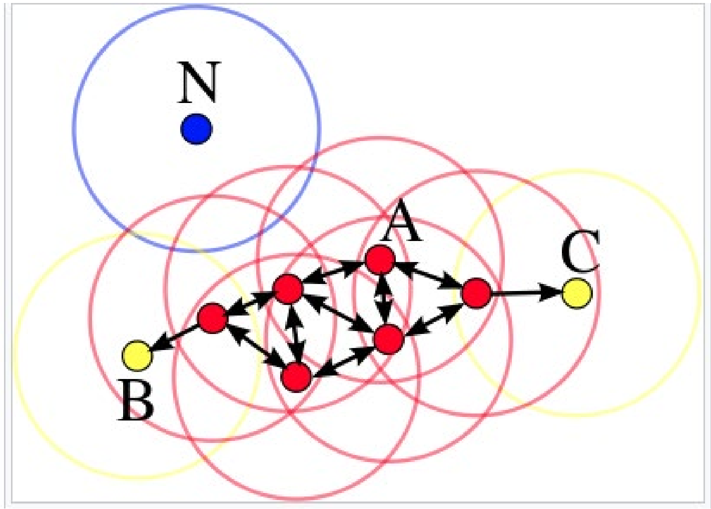
找出所有核心对象

随机选一个核心对象生长出一个簇，并在核心对象集合里删去该核心对象

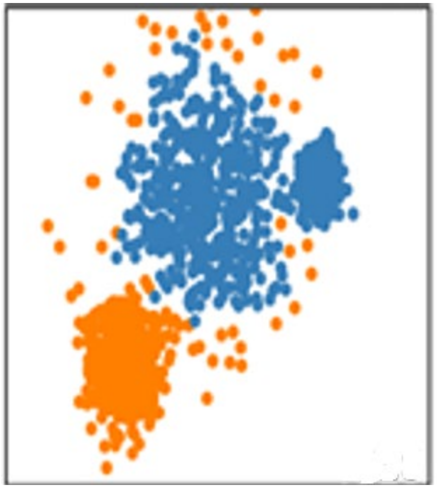
DBSCAN

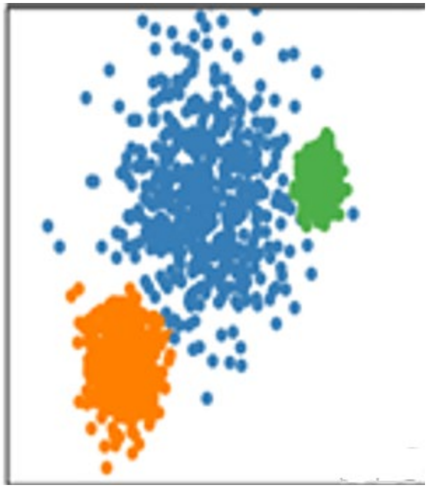
- Strengths
  - There is no K.
  - It can discover any shape of spatial clustering.
  - It can discard the remote point.



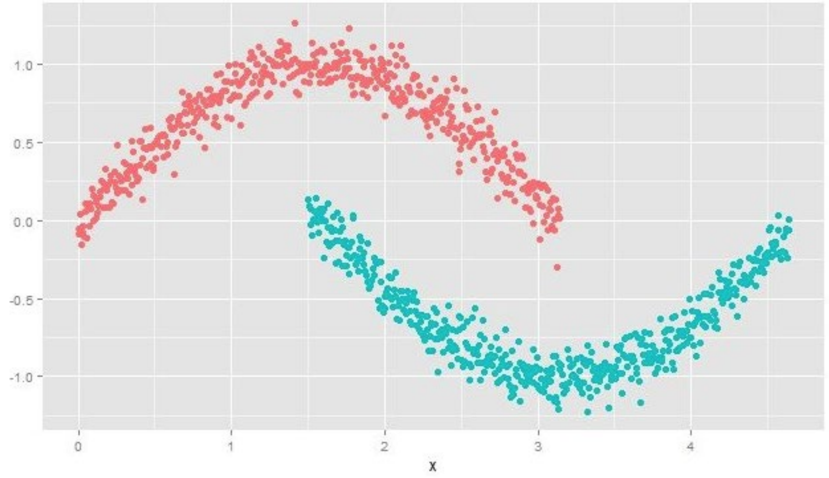


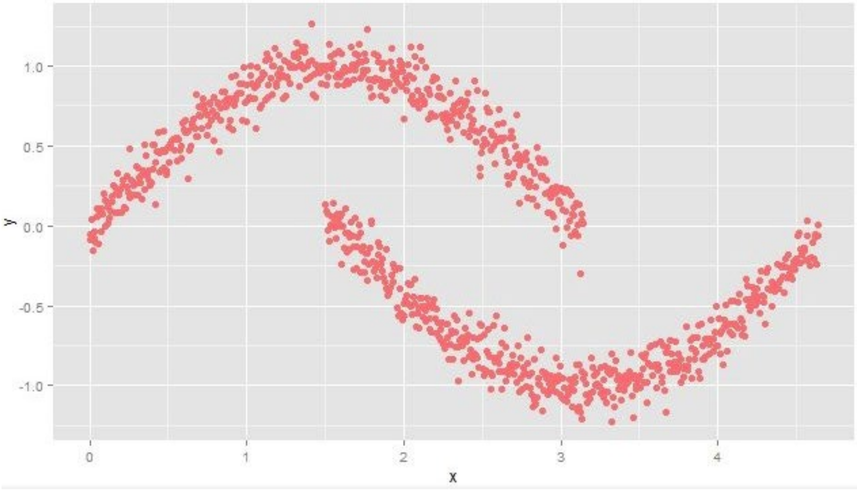
- Weaknesses
  - It is not suitable when the cluster spacing difference is very different.
  - Parameters adjustment are more complicated.





AGNES

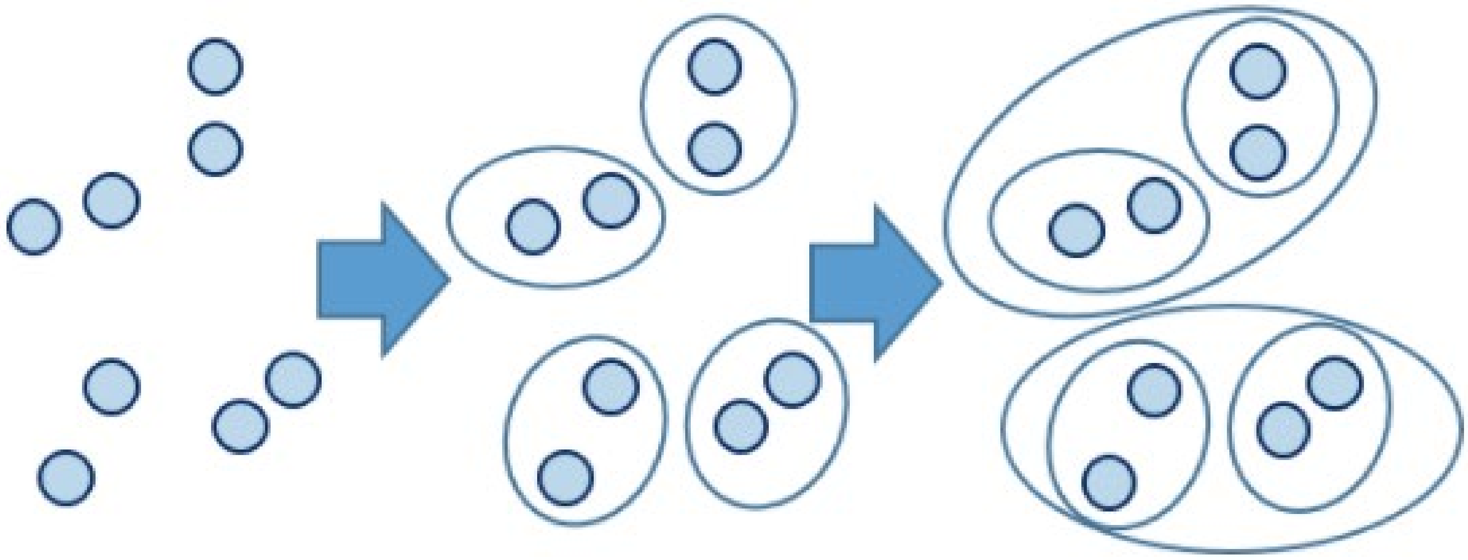




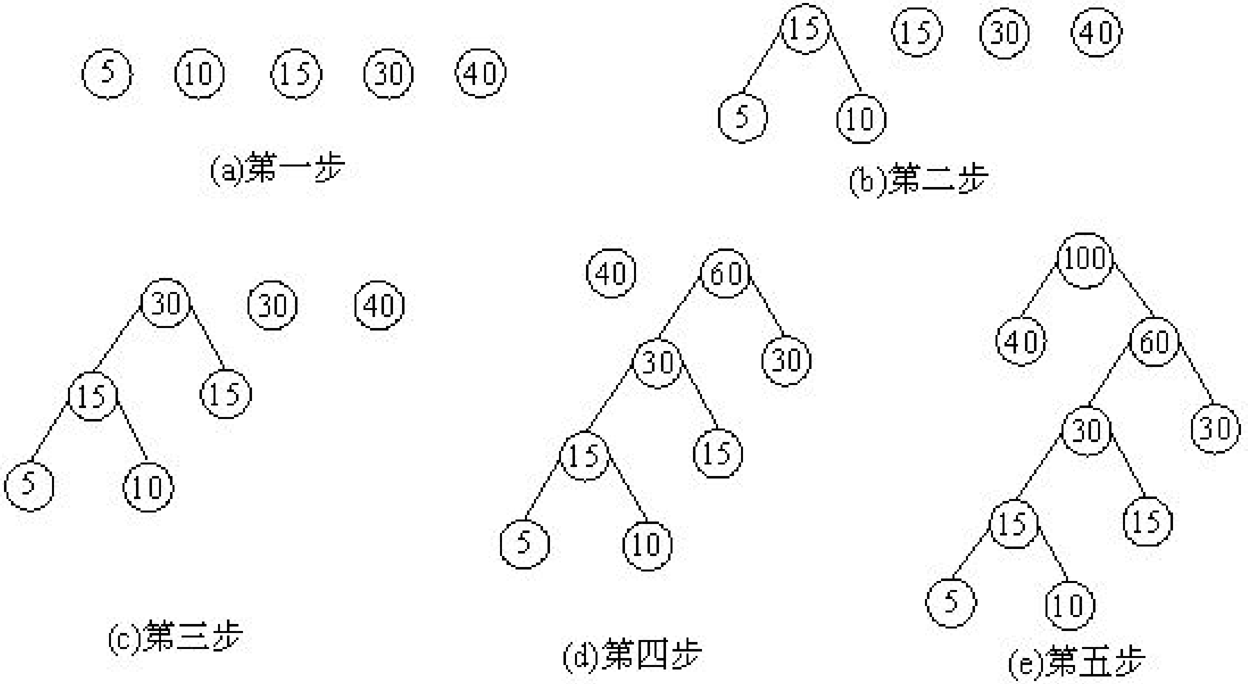
AGNES

MIMA

- AGNES is a kind of Hierarchical clustering



AGNES



(a)第一步

(b)第二步

(c)第三步

(d)第四步

(e)第五步

AGNES

- Given cluster C_i , C_j, Usually the distance between two clusters is one of the following
  - Maximum distance(also called complete-linkage clustering)

$$dist_{max}(C_i , C_j) = \max_{x \in C_i , z \in C_j} dist(x, z)$$

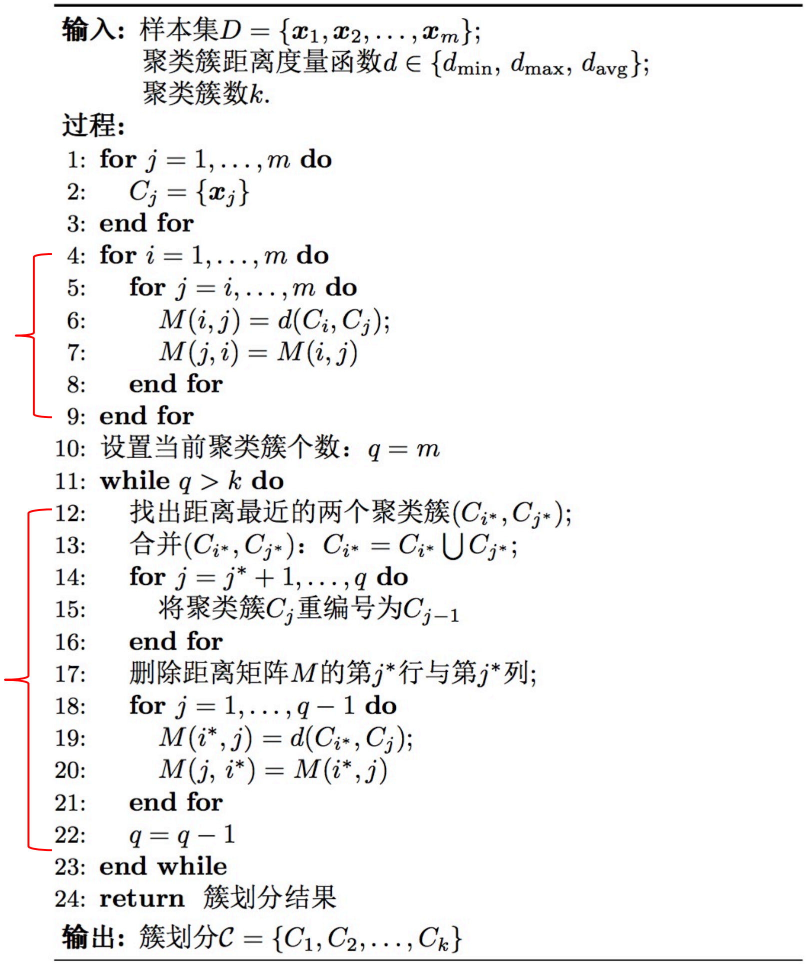
  - Minimum distance(also called single-linkage clustering)

$$dist_{\min}(C_i , C_j) = \min_{x \in C_i , z \in C_j} dist(x, z)$$

  - Average distance (also called average-linkage clustering)

$$dist_{avg}(C_i , C_j) = \frac{1}{|C_i||C_j|} \sum_{x \in C_i} \sum_{z \in C_j} dist(x, z)$$

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$d \in \{d_{\min}, d_{\max}, d_{\text{avg}}\}$;
      聚类簇数$k$.
过程:
for $j = 1, \ldots, m$ do
    $C_j = \{\boldsymbol{x}_j\}$
end for
for $i = 1, \ldots, m$ do
    for $j = i, \ldots, m$ 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$(C_{i^*}, C_{j^*})$;
    合并$(C_{i^*}, C_{j^*})$: $C_{i^*} = C_{i^*} \bigcup C_{j^*}$;
    for $j = j^* + 1, \ldots, q$ 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 $j = 1, \ldots, q - 1$ do
        $M(i^*, j) = d(C_{i^*}, C_j)$;
        $M(j, i^*) = M(i^*, j)$
    end for
    $q = q - 1$
end while
return 簇划分结果
输出: 簇划分$\mathcal{C} = \{C_1, C_2, \ldots, C_k\}$
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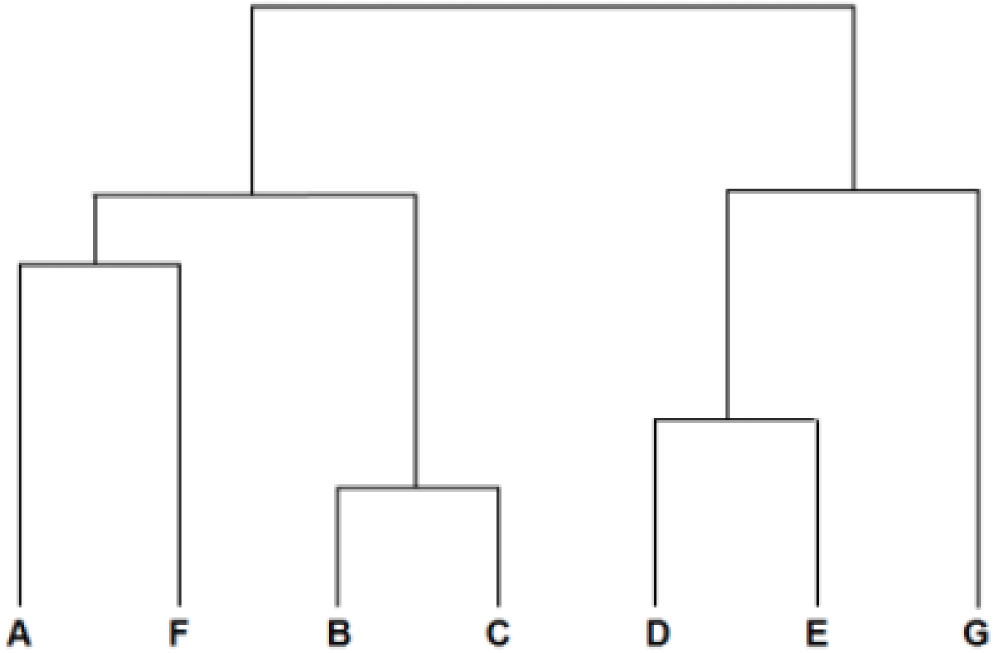
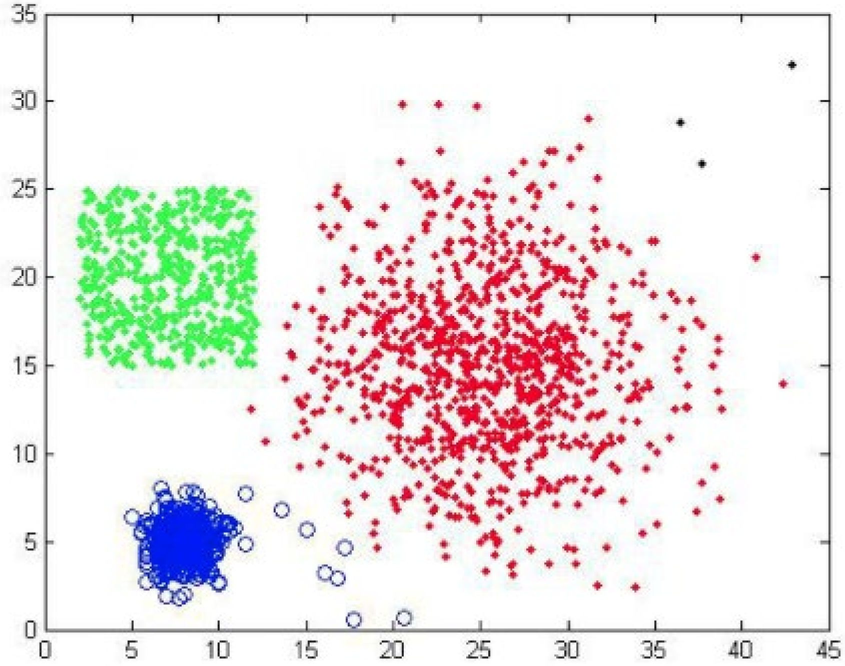
计算距离矩阵

每次循环合并两个簇并更新距离矩阵


A
F
B
C
D
E
G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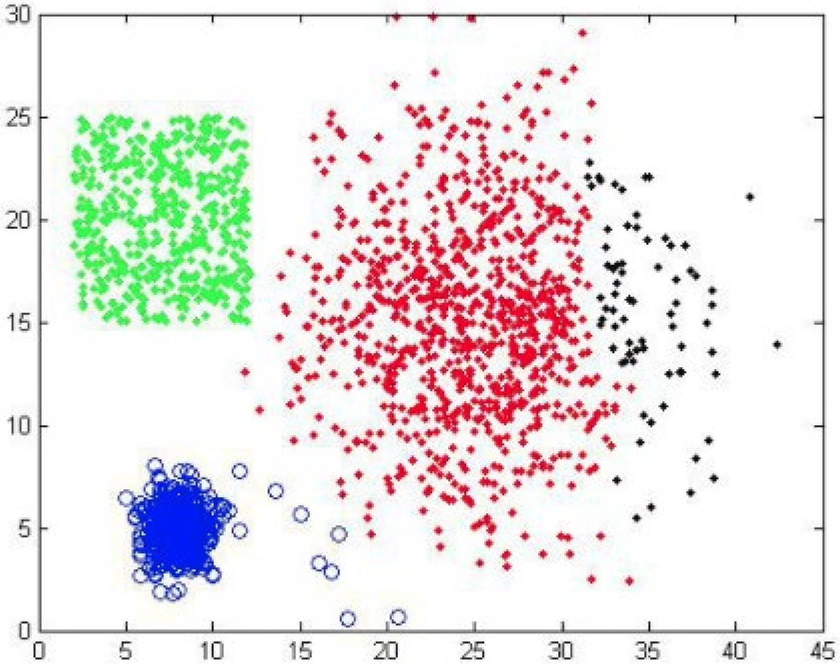
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- Partitioning Methods
  - k-means, k-medoids, CLARANS, FCM
- Hierarchical Methods
  - AGNES, Birch, Cure, Rock, CHEMALOEN
- Density-based Methods
  - DBSCAN,OPTICS
- Grid-based Methods
- Model-Based Methods
  - Transitive closure, Boolean matrix, direct clustering, correlation analysis clustering, clustering method based on statistics……

Performance Measurement

- Good clustering should be:

Intra-cluster similarity ⇨ maximized

Inter-cluster similarity ⇨ minimized

Intra distance & Inter distance

Intra distance

$$agv(C) = \frac{2}{|C|(|C|-1)} \sum_{1 \le i \le j \le |C|} dist(x_i, x_j)$$

$$diam(C) = \max_{1 \le i \le j \le |C|} dist(x_i, x_j)$$

Inter distance

$$d_{min}(C_i, C_j) = \min_{x_i \in C_i, x_j \in C_j} dist(x_i, x_j)$$

$$d_{cen}(C_i, C_j) = dis(\mu_i, \mu_j)$$

Performance Measurement

- Internal Index
  - Evaluate clustering results directly without using reference model.

- External Index
  - Compare clustering results with reference model, for example, partitioning results given by domain expert.

Internal Index

- Davies-Boukdin Index:

The smaller the better

$$DBI = \frac{1}{k}\sum_{i=1}^{k}\boxed{\max_{j\neq i}\boxed{\left(\frac{avg(C_i)+avg(C_j)}{d_{cen}(C_i,C_j)}\right)}}$$

- Dunn Index:

The bigger the better

$$DI = \min_{1\leq i\leq k}\boxed{\left\{\min_{j\neq i}\boxed{\frac{d_{min}(C_i,C_j)}{\max\limits_{1\leq l\leq k} diam(C_l)}}\right\}}$$

External Index

- Assume our cluster partition is
  - $C = \{C_1, C_2, \dots C_k\}$
- The partition given by reference model is
- $C^* = \{C_1^*, C_2^*, \dots C_s^*\}$
- let $\boldsymbol{\lambda}$ and $\boldsymbol{\lambda}^*$ be clustering label vectors corresponding to
- C and C^*. Consider C_m^2 sample pairs
- $$a = |SS|, SS = \{(x_i, x_j) | \lambda_i = \lambda_j, \lambda_i{}^* = \lambda_j{}^*, i < j\}$$
  $$b = |SD|, SS = \{(x_i, x_j) | \lambda_i = \lambda_j, \lambda_i{}^* \neq \lambda_j{}^*, i < j\}$$
  $$c = |DS|, SS = \{(x_i, x_j) | \lambda_i \neq \lambda_j, \lambda_i{}^* = \lambda_j{}^*, i < j\}$$
  $$d = |DD|, SS = \{(x_i, x_j) | \lambda_i \neq \lambda_j, \lambda_i{}^* \neq \lambda_j{}^*, i < j\}$$
  $$a + b + c + d = C_m^2 = m(m-1)/2$$

External Index

- JC: Jaccard Coefficient

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

- FMI: Fowlkes and Mallows Index

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

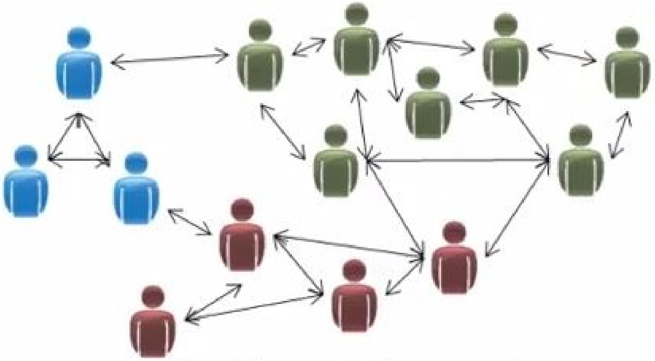
- RI: Rand Index

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

[0,1] interval
the bigger
the better

Applications

Organize computing clusters



Social network analysis

Market segmentation

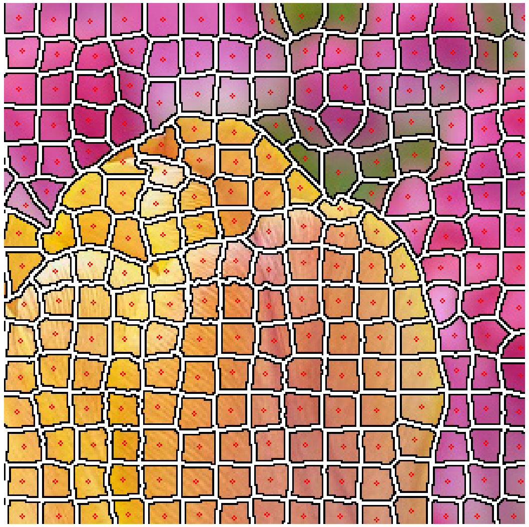
Image credit: NASA/JPL-Caltech/E. Churchwell (Univ. of Wisconsin, Madison)

Astronomical data analysis

An Example

MIMA

- Superpixel segmentation uses the similarity of features between pixels to group pixels, and replaces a large number of pixels with a small number of superpixels to express image features.



【 Thank You ! 】

Any Question?