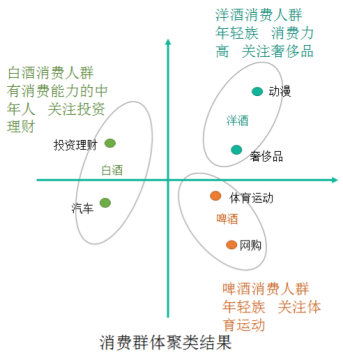
Clustering

- Also called data segmentation, group a collection of objects into subsets or "clusters"
- Results : objects in each cluster are more similar to one another than objects in different clusters.
- Example : applications in consumption analysis
- Can be used in data preprocessing



消费群体聚类结果

将样本聚分成几类

可用于数据预处理

Concepts in Clustering

- Different from classification : it is unsupervised learning ; no outputs or labels
- Central goal : Optimize the similarity (or dissimilarity) between the individual objects being clustered :
  - Obtain great similarity of samples within cluster
  - Obtain small similarity of samples between clusters
- Cost functions : not related to the outputs, but related to the similarity
- Two kinds of input data :
  - $n \times n$ similarity (dissimilarity) matrix D : only depends on the distances between pairs of samples ; may lose some information on data
  - Original data with features $X \in \mathbb{R}^{n \times d}$

无监督学习、无 Label 和输出.

相似度高 → 同簇

相似度低 → 不同簇

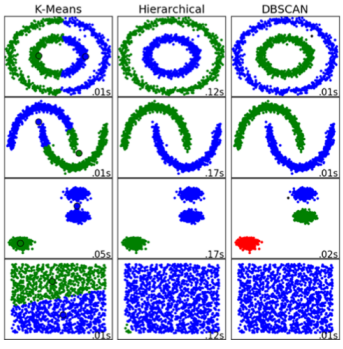
cost function：与输出无关，与相似度有关.

相似度矩阵：两两之间的相似度

连续型数据用距离代替.

Clustering Methods

- Clustering process :
  - data preprocessing, especially standadization
  - Similarity matrix
  - Clustering Methods
  - Determine the best number of clusters
- Clustering methods :
  - Partitional clustering :
    - K-means
    - K-Medoids
    - Spectral clustering
    - DBSCAN
  - Hierarchical clustering



K-Means

Introduction

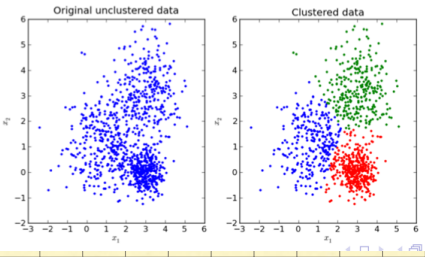
- K-means clustering originates from signal processing, it is quite popular in image processing (segmentation)
- Group n samples to k clusters, making each sample belong to the nearest cluster
- In an image, each pixel is a sample

将n个样本分到k个簇中.

Idea

若样本在欧氏空间的形状是凸的，用k-Means比较好.
重心得到划分到同一簇中的点离重心最近.

- Data set $\{\mathbf{x}_i\}_{i=1}^n$, $\mathbf{x}_i \in \mathbb{R}^d$
- Representatives : Mass center of kth-cluster C_k is c_k, $k = 1, \ldots, K$
- Sample x_i belongs to cluster k if $d(x_i, c_k) < d(x_i, c_m)$ for $m \neq k$, where $d(x_i, x_j)$ is dissimilarity function
- Make the mass centers well-located so that the average distance between each sample to its cluster center is as small as possible



Optimization Problem

- Let $C : \{1, \ldots, n\} \to \{1, \ldots, k\}$ be the assignment from the data indices to the cluster indices. $C(i) = k$ means $x_i \in C_k$
- Total point scatter : $T = \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} d(x_i, x_j) =$ 任意两点之间的距离

$$\frac{1}{2} \sum_{k=1}^{K} \sum_{C(i)=k} \left(\sum_{C(j)=k} d_{ij} + \sum_{C(j)\neq k} d_{ij} \right) = W(C) + B(C)$$

- Loss function : within-cluster point scatter

$W(C) = \frac{1}{2} \sum_{k=1}^{K} \sum_{C(i)=k} \sum_{C(j)=k} d_{ij}$; between-cluster point scatter

$B(C) = \frac{1}{2} \sum_{k=1}^{K} \sum_{C(i)=k} \sum_{C(j)\neq k} d_{ij}$

- Minimize $W(C)$ is equivalent to maximize $B(C)$

Dissimilarities

- Proximity matrices : $n \times n$ symmetric matrix D with nonnegative entries and zero diagonal elements provides information about dissimilarity between a pair of samples, this is not distance in general
- Dissimilarities based on attributes :
  $d(x_i, x_j) = \sum_{k=1}^{p} d_k(x_{ik}, x_{jk})$; d_k can be squared distance $d_k(x_{ik}, x_{jk}) = (x_{ik} - x_{jk})^2$, absolute distance $d_k(x_{ik}, x_{jk}) = |x_{ik} - x_{jk}|$
- Weighted average : $d(x_i, x_j) = \sum_{k=1}^{p} w_k d_k(x_{ik}, x_{jk})$ where $\sum_{k=1}^{p} w_k = 1$; setting $w_k \sim 1/\bar{d}_k$ with $\bar{d}_k = \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} d_k(x_{ik}, x_{jk}) = 2\widehat{\mathrm{Var}}(X_k)$ will assign equal influence to all features
- Dissimilarities based on correlation : $d(x_i, x_j) \propto 1 - \rho(x_i, x_j)$

K-Means (as Central Voroni Tessellation)

- Minimizing $W(C)$ is in general infeasible since this is a greedy algorithm that only works for small data sets
- Taking squared dissimilarity, $W(C) = \sum_{k=1}^{K} n_k \sum_{C(i)=k} \|x_i - \bar{x}_k\|^2$, where $n_k = \sum_{i=1}^{n} I(C(i) = k)$ is the number of samples in cluster k, $\bar{x}_k = \frac{1}{n_k} \sum_{C(j)=k} x_j = \arg\min_{m_k} \sum_{C(j)=k} \|x_j - m_k\|^2$
- $\min_C W(C) \Longleftrightarrow \min_{C, m_k} \sum_{k=1}^{K} n_k \sum_{C(i)=k} \|x_i - m_k\|^2$
- Alternating minimization :
  1. Given C, solve for $m_k \Longrightarrow m_k^* = \bar{x}_k$ (choose representatives)
  2. Given m_k, solve for $C \Longrightarrow C(i) = \arg\min_{1 \leqslant k \leqslant K} \|x_i - m_k\|^2$ (partitioning, equivalent to Voronoi tessellation for given center m_k)

$$W(C) = \frac{1}{2} \sum_{k=1}^{K} \sum_{C(i)=k} \sum_{C(j)=k} d(x_i, x_j)$$

$$= \frac{1}{2} \sum_{k=1}^{K} \sum_{C(i)=k} \sum_{C(j)=k} \|x_i - x_j\|_2^2$$

$\|x_i\|_2^2 - 2x_i x_j + \|x_j\|_2^2$ 求和后 i 和 j 会重复

$$= \sum_{k=1}^{K} \left(\sum_{C(i)=k} \sum_{C(j)=k} \|x_i\|_2^2 - \sum_{C(i)=k} \sum_{C(j)=k} x_i x_j \right)$$

$N_k = \sum_{C(j)=k} 1$ = #{cluster k}

$\bar{x}_k = \frac{1}{N_k} \sum_{C(j)=k} x_j$

$$= \sum_{k=1}^{K} \left(\sum_{C(i)=k} x_i \left(\sum_{C(j)=k} x_i - \sum_{C(j)=k} x_j \right) \right)$$

$N_k x_i - N_k \bar{x}_k$

$$= \sum_{k=1}^{K} N_k \sum_{C(i)=k} \|x_i - \bar{x}_k\|_2^2$$

$$= \sum_{k=1}^{K} N_k \min_{m_k} \sum_{C(i)=k} \|x_i - m_k\|_2^2$$

$$= \min_{\{m_1, m_2, \cdots, m_K\}} \sum_{k=1}^{K} N_k \sum_{C(i)=k} \|x_i - m_k\|_2^2$$

$$\min_C W(C) = \min_C \min_{\{m_k\}} \sum_{k=1}^{K} N_k \sum_{C(i)=k} \|x_i - m_k\|_2^2$$

① Given C, solve $\{m_k\}$. $m_k = \bar{x}_k = \frac{1}{N_k} \sum_{C(i)=k} x_i$

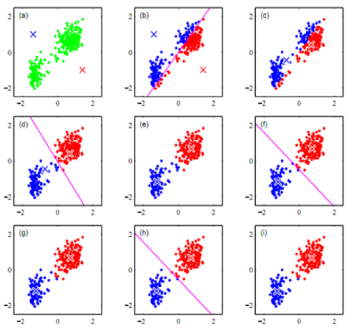
② Given $\{m_k\}$, solve C. $C(i) = \min_k \|x_i - m_k\|_2^2$

①、②交替迭代

这是种贪心算法，没有全局最小，初始值选择很重要

K-Means Iterations

- The alternating iterations can stop when the mass centers $\{\bar{x}_k\}_{k=1}^{K}$ do not change
- Initial guess :
  - Random guess, try the best one with smallest $W(C)$
  - Base on other clustering methods (e.g., hierarchical clustering), choose the cluster centers as initial guess



直到代表元(重心)不变时停止

(可能不收敛，重心不断变动)

二分聚类比较容易收敛.

How to choose K

- Minimizing Bayesian Information Criterion (BIC) : $BIC(\mathcal{M}|\mathbf{X}) = -2 \log \Pr(\mathbf{X}|\hat{\Theta}, \mathcal{M}) + p \log(n)$, where $\mathcal{M}$ indicates the model, $\hat{\Theta}$ is the MLE of the model parameters in $\mathcal{M}$, $\Pr(\mathbf{X}|\mathcal{M})$ is the likelihood function, and p is the number of parameters in model $\mathcal{M}$; trade-off between log-likelihood and model complexity

依赖于模型

平衡于 log-likelihood 和模型复杂度.

- Based on Minimum Description Length (MDL) : starting from large K, decreases K until the description length $-\log \Pr(\mathbf{X}|\hat{\Theta}, \mathcal{M}) - \log \Pr(\Theta|\mathcal{M})$ achieves its minimum (similar to MAP)

从 $K=1$ 开始不断增大，直至每个簇中的点符合高斯分布

- Based on Gaussian distribution assumption : starting from $K = 1$, increases K until the points in every cluster follow Gaussian distribution

Pros and Cons

- Where it is good
  - Intuitive, easy to implement
  - Low computational complexity, $O(tnpK)$, where t is the number of iterations

复杂度与K近邻类似.

- Disadvantage
  - Need to specify K first (K is tuning parameter)
  - Strong dependence on the initial guess of cluster center
  - Easy to stuck at local minimum
  - Naturally assume ball-shaped data, hard to deal with data which are not ball-shaped
  - Sensitive to outliers

容易卡在局部最优

对异常值敏感

Variant : Bisecting K-Means

每次都二分

- Invented to deal with initial guess of center selection
- Idea : sequentially divide the poorest cluster into two sub-clusters
  1. Initially gather all data into one cluster
  2. Repeat :
     - 2.1 Select the cluster k that maximizes the within-cluster point scatter $\sum_{C(i)=k} \sum_{C(j)=k} \|x_i - x_j\|^2$
     - 2.2 Use 2-means to divide cluster k into two sub-clusters, with random initial guess of two centers
     - 2.3 Repeat step 2.2 p times, choose the best pair of clusters that minimizes the within-cluster point scatter
  3. Stop when there are K clusters (Or you can stop any time you like to have a satisfactory clustering result)

Variant : K-medoids

- Invented to overcome the influence of outliers
- Can deal with data of general type, assuming general dissimilarity $d(x_i, x_j)$
- Idea : centers for each cluster are restricted to be one of the observations assigned to that cluster
- Alternating minimization :
  1. Given C, solve for $m_k = x_{i_k^*}$ that minimizes the within-cluster point scatter : $i_k^* = \arg \min_{\{i:C(i)=k\}} \sum_{C(j)=k} d(x_i, x_j)$ (choose the real samples as representatives)
  2. Given m_k, solve for $C \implies C(i) = \arg \min_{1 \leqslant k \leqslant K} d(x_i, m_k)$
- More robust than K-means
- More computational effort when solving for the center in step 1 : $O(n_k^2)$ comparing to $O(n_k)$ in K-means

Other Variants

- K-medians : use Manhattan distance (L^1-distance) instead in K-means; then the centers are not means, but medians
- K-means++ : designed to select good initial centers that are far away from each other
- Rough-set-based K-means : each sample could be assigned to more than one cluster

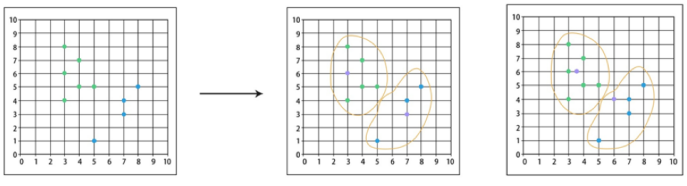


FIGURE: K-medoids

Hierarchy Clustering 层次聚类

- Clustering in different hierarchies, generating tree structure
- Two approaches :
  - Agglomerate clustering : bottom-up
  - Divisive clustering : top-down
- Limitation : once merged or divided, the operation cannot be modified

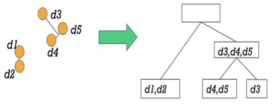


FIGURE: Agglomerate clustering

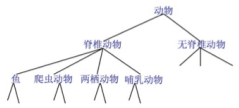


FIGURE: Divisive clustering

在不同层级上对样本聚类，逐步形成树状的结构.
① 自下而上：聚合方法 } 两种方法，均无明确
② 自上而下：分拆方法 } 的目标函数来实现

一旦分出合入某个节点，就再也不能修改了.

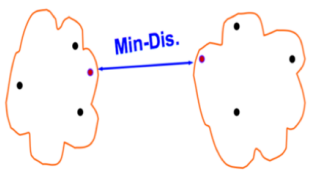
Agglomerate Clustering

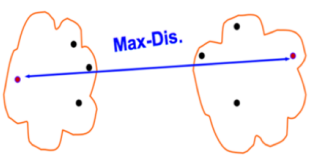
- Given n samples and proximity matrix, do the following steps :
  1. Let every observation represent a singleton cluster
  2. Merge the two closest clusters into one single cluster
  3. Calculate the new proximity matrix (dissimilarity between two clusters)
  4. Repeat step 2 and 3, until all samples are merged into one cluster
- Three methods for computing intergroup dissimilarity :
  - Single linkage (SL)
  - Complete linkage (CL)
  - Average linkage (AL)

开始时将每个样本都当成一个簇，
每次迭代时将最相似的两个簇合并.
直到最终所有簇合并成一个含有所有样本的簇.
复杂度 $O(n^3)$，用优先队列优化 $O(n^2 \ln n)$

Intergroup Dissimilarity

- Single linkage : Greatest similarity or least dissimilarity $d_{SL}(C_i, C_j) = \min_{x \in C_i, y \in C_j} d(x, y)$
- Complete linkage : Least similarity or greatest dissimilarity $d_{SL}(C_i, C_j) = \max_{x \in C_i, y \in C_j} d(x, y)$
- Average linkage : Average similarity or dissimilarity $d_{AL}(C_i, C_j) = \frac{1}{|C_i||C_j|} \sum_{x \in C_i, y \in C_j} d(x, y)$





单连接：C_i 和 C_j 中最近两点的距离

完整连接：C_i 和 C_j 中最远两点的距离

平均连接：C_i 和 C_j 中所有成员对的平均距离.

Generalized Agglomerative Scheme

- Input : training set $D = \{(x_1), \ldots, (x_n)\}$, dissimilarity function $d(C_i, C_j)$
- Output : A dendrogram containing $\{\mathcal{R}_t\}_{t=0}^{n-1}$, where $\mathcal{R}_t$ is the clustering result at time t

1. Initialize the clustering result $\mathcal{R}_0 = \{\{x_1\}, \{x_2\}, \ldots, \{x_n\}\}$, $t = 0$
2. Do iterations :
   - 2.1 $t = t + 1$
   - 2.2 Choose (C_i, C_j) from $\mathcal{R}_{t-1}$ so that $d(C_i, C_j) = \min_{(r,s)} d(C_r, C_s)$
   - 2.3 $C_q = C_i \bigcup C_j$
   - 2.4 $\mathcal{R}_t = (\mathcal{R}_{t-1} \setminus \{C_i, C_j\} \bigcup \{C_q\})$
3. Stop at $t = n - 1$ when $|\mathcal{R}_{n-1}| = 1$, return $\{\mathcal{R}_t\}_{t=0}^{n-1}$

Generalized Divisive Scheme

- Input : training set $D = \{(x_1), \ldots, (x_n)\}$, dissimilarity function $d(C_i, C_j)$
- Output : A dendrogram containing $\{\mathcal{R}_t\}_{t=0}^{n-1}$, where $\mathcal{R}_t = \{C_{t,i}\}_{i=1}^{t+1}$ is the clustering result at time t

1. Initialize $\mathcal{R}_0 = \{X\}$, $t = 0$
2. Do iterations :
   - 2.1 $t = t + 1$
   - 2.2 For $i = 1$ to t, do :
     - 2.2.1 Choose $(C_{t-1,i}^1, C_{t-1,i}^2)$ from $C_{t-1,i}$ so that $d(C_{t-1,i}^1, C_{t-1,i}^2) = \max_{G \bigcup H = C_{t-1,i}} d(G, H)$
   - 2.3 Choose i_{t-1} so that $i_{t-1} = \arg\max_i d(C_{t-1,i}^1, C_{t-1,i}^2)$
   - 2.4 $\mathcal{R}_t = (\mathcal{R}_{t-1} \setminus \{C_{t-1,i_{t-1}}\}) \bigcup \{C_{t-1,i}^1, C_{t-1,i}^2\})$
3. Stop at $t = n - 1$ when $|\mathcal{R}_{n-1}| = n$, return $\{\mathcal{R}_t\}_{t=0}^{n-1}$

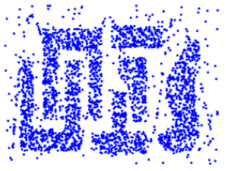
Pros and Cons

- Where it is good
  - Hierarchical clustering computes tree structure of the whole clustering process in one stroke
  - SL and CL are sensitive to outliers, while AL gives a compromise
    - As $n \to \infty$, $d_{AL}(C_i, C_j) \to \int\int d(x, y) p_i(x) p_j(y) \mathrm{d}x\mathrm{d}y$, the expected dissimilarity w.r.t. the two densities $p_i(x)$ and $p_j(x)$
    - In contrast, $d_{SL}(C_i, C_j) \to 0$ and $d_{CL}(C_i, C_j) \to \infty$ independent of $p_i(x)$ and $p_j(x)$
- Disadvantage
  - Computationally intensive
  - Once a sample is incorrectly grouped into a branch, it will stay in the clusters corresponding to that branch no matter how you threshold the tree

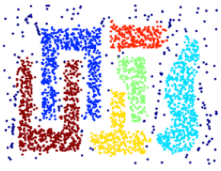
一般用于预判.
层次聚类的空间/时间复杂度均高于K-Means

Density-based Clustering

- Limitations of hierarchical clustering and K-means clustering : tend to discover convex clusters
- Density-based Clustering : looks for high-density regions separated by low-density regions, could discover clusters of any shape
- Density-Based Spatial Clustering of Applications with Noise (DBSCAN)



Original Points



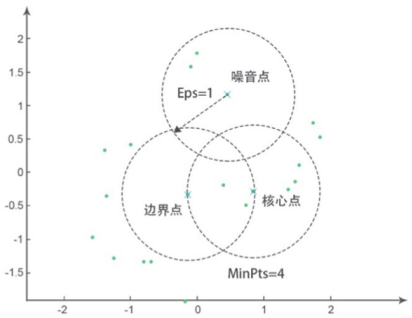
Clusters

层次聚类和K-means聚类都趋向于找到凸聚类.

密度聚类：用低密度区域作为分割线.

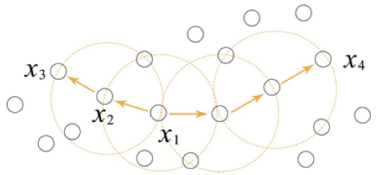
Concepts

- Three types of points :
  - Core point : # of samples in its ϵ-neighborhood $\geqslant$ MinPts
  - Boundary point : it lies in the ϵ-neighborhood of some core point, # of samples in its ϵ-neighborhood $<$ MinPts
  - Noise point : neither core point nor boundary point, it lies in the sparse region



核心点：该点的ε近邻数≥最小点数.
边界点：在某个核心点的ε近邻内.但该点的ε近邻数<最小点数.
噪音点：既非核心点又非噪音点.

- ϵ-neighborhood : for each sample $x_i \in D$, $N_\epsilon(x_i) = \{x_j \in D | d(x_i, x_j) \leqslant \epsilon\}$
- Directly density-reachable : if the sample $x_j \in N_\epsilon(x_i)$, and x_i is core point, then x_j is directly density-reachable from x_i
- Density-reachable : for x_i and x_j, if there exist $p_1, \ldots, p_m$, s.t. $p_1 = x_i, p_m = x_j$, and p_{k+1} is directly density-reachable from p_k, then x_j is density-reachable from x_j
- Density-connected : if there exists p, s.t. both x_i and x_j are density-reachable from p, then x_i and x_j are density-connected



密度直达：①出发点是核心点
②终点在核心点的邻域.

密度可达：有一条道路连接.

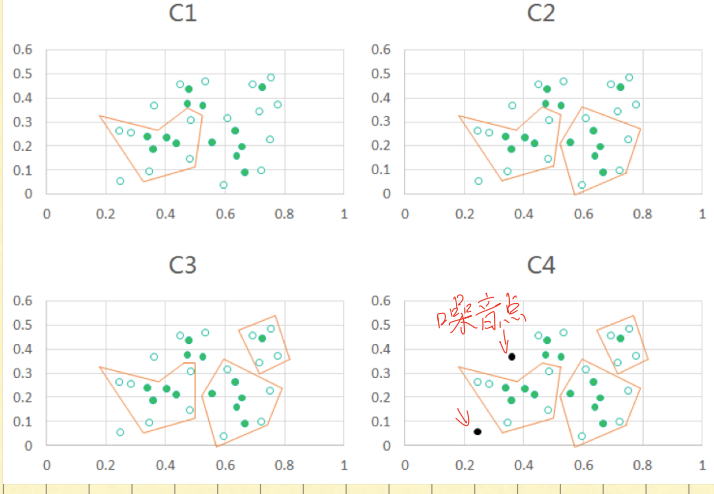
密度连通：两点分别能密度可达到第三个点.

DBSCAN Algorithm

- Input : training set $D = \{(x_1), \ldots, (x_n)\}$, dissimilarity function $d(C_i, C_j)$, parameters $MinPts, \epsilon$
- Output : a set of clusters $\{C_t\}$

1. Mark all samples in D as non-processed
2. For each sample $p \in D$, do :
   - 2.1 If p has been grouped into some cluster or marked as noise point, go to check next sample
   - 2.2 Else, if $|N_\epsilon(p)| < MinPts$, then mark p as boundary point or noise point
   - 2.3 Else, mark p as core point, construct cluster $C = N_\epsilon(p)$. For each $q \in N_\epsilon(p)$, do :
     - 2.3.1 If $|N_\epsilon(q)| \geqslant MinPts$, then put all un-clustered points in $N_\epsilon(q)$ into C
3. Stop when all samples in D have been clustered

Example ($\epsilon = 0.11$, $MinPts = 5$)



噪音点不一定是outlier.
可以调整MinPts或距离计算方法. 若仍是噪音点，则很可能是outlier.

DBSCAN vs. K-means

DBSCAN

- The clustering result is not a complete partition of original dataset (noise points are excluded)
- Could deal with clusters with any shape and size
- Could deal with noise points and outliers
- The definition of density must be meaningful
- Not efficient when dealing with high-dimensional data
- No implicit assumptions on the sample distribution

K-Means

- The clustering result is a complete partition of original dataset
- The clusters are nearly ball-shaped
- Sensitive to outliers
- The definition of cluster centers must be meaningful
- Efficient to deal with high-dimensional data
- The samples implicitly follow the Gaussian distribution assumption

DBSCAN没有依赖于任何假设，形状不一.

Pros and Cons

- Computational complexity $O(n \times T)$, where T is the time for searching ϵ-neighborhood); in the worst case, $O(n^2)$
- In low-dimensional space, could be improved as $O(n \log n)$ by KD-tree
- Where it is good
  - Fast for clustering
  - Better to deal with noise points
  - Effective for clusters of any shape
- Disadvantage
  - Need large memory
  - Bad performance when the density is not well-distributed and the between-cluster distances are large

做聚类很快
对噪音点处理得好.

需要大内存
对点的密度分布不好的和簇间距大的效果不好.

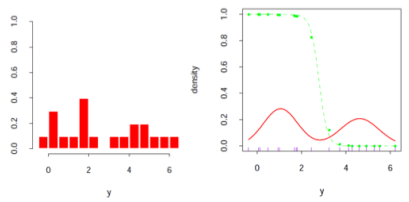
Expectation-Maximization Algorithm (一般是生成模型)

Gaussian Mixture Models

无监督

- We want to estimate the density of given data set. This is an unsupervised learning problem.
- Commonly used approach is the parametric estimation, such as maximum likelihood estimate (MLE).
- Consider the following set of data points :

-0.39	0.12	0.94	1.67	1.76	2.44	3.72	4.28	4.92	5.53
0.06	0.48	1.01	1.68	1.80	3.25	4.12	4.60	5.28	6.22



Latent Variables 隐变量

将两个符合高斯分布的变量加权合并，形成一个新变量.

- A single Gaussian family would not be appropriate. A mixture of two Gaussian distributions seems good.

$$Z_1 \sim N(\mu_1, \sigma_1^2), \quad Z_2 \sim N(\mu_2, \sigma_2^2), \quad Z = (1 - Y)Z_1 + YZ_2,$$

  where $Y \in \{0, 1\}$ with $P(Y = 1) = c$.
- In general, for mixture of K Gaussian distributions, we assume there is a latent variable Y indicating which distribution the data $\mathbf{x}$ is sampled from, i.e., $P(Y = y) = c_y$ with $y \in \{1, \ldots, K\}$. Given $Y = y$, the random variable X follows the conditional distribution :

$$P(X = \mathbf{x}|Y = y) = \frac{1}{(2\pi)^{d/2}(\Sigma_y)^{1/2}} \exp\Big(-\frac{1}{2}(\mathbf{x}-\mu_y)^T\Sigma_y^{-1}(\mathbf{x}-\mu_y)\Big).$$

- The density of X is then

$$\begin{aligned} P(X = \mathbf{x}) &= \sum_{y=1}^{K} P(Y = y)P(X = \mathbf{x}|Y = y) \\ &= \sum_{y=1}^{K} c_y \frac{1}{(2\pi)^{d/2}(\Sigma_y)^{1/2}} \exp\Big(-\frac{1}{2}(\mathbf{x} - \mu_y)^T\Sigma_y^{-1}(\mathbf{x} - \mu_y)\Big). \end{aligned}$$

MLE of Gaussian Mixture

- Let $\theta = (c_y, \mu_y, \Sigma_y)_{y=1}^K$. Then the log-likelihood of the sample set $S = \{\mathbf{x}_i\}_{i=1}^n$ is

$$L(\theta) = \sum_{i=1}^n \log P_\theta(X = \mathbf{x}_i) = \sum_{i=1}^n \log \Big(\sum_{y=1}^K P_\theta(X = \mathbf{x}_i, Y = y) \Big).$$

- MLE : $\theta = \arg\max_\theta L(\theta)$ is hard due to the summation inside the log.
- Make a simple assumption : we have known the value of the latent variable for each sample $\mathbf{x}_i$, i.e., $Y_i \in \{1, \dots, K\}$ is known, then the choice from the Y_i-th Gaussian becomes deterministic, and the log-likelihood is replaced by

这个求和在这里只有一个分量

$$\tilde{L}(\theta) = \sum_{i=1}^n \log \Big(\sum_{y=1}^K I_{(Y_i=y)} P_\theta(X = \mathbf{x}_i, Y = y) \Big)$$

$$= \sum_{i=1}^n \sum_{y=1}^K I_{(Y_i=y)} \log P_\theta(X = \mathbf{x}_i, Y = y).$$

$Y_i=y$ 满足一个分布.

可用梯度下降法直接解: $\theta^{(m+1)} = \theta^{(m)} - \alpha \nabla_\theta (-L(\theta))$

由于log内有求和,比较难算.

对每个Y_i,它要么是0要么是1

也可以用琴生不等式.

Expectation-Maximization (EM) Algorithm (Dempster, Laird, and Rubin, 1977)

若$Y_i=y$服从一个分布.

- But Y_i is indeed random, so that the event $Y_i = y$ happens with a probability $Q_{i,y}$ with $\sum_{y=1}^k Q_{i,y} = 1$.
- Consider the modified objective function defined over $Q = (Q_{i,y})_{i=1,\dots,n;y=1,\dots,K}$ and θ

与L不是一个

$$F(Q, \theta) = \sum_{i=1}^n \sum_{y=1}^K Q_{i,y} \log \Big(P_\theta(X = \mathbf{x}_i, Y = y) \Big).$$

- The optimization problem $(Q, \theta) = \arg\max_{Q,\theta} F(Q, \theta)$ can be solved alternatingly :
  1. E-Step : Given $\theta^{(m)}$, solve for $Q^{(m+1)} = E_{\theta^{(m)}}(I_{(Y=y)}|X = \mathbf{x}_i) = P_{\theta^{(m)}}(Y = y|X = \mathbf{x}_i)$; (用上一步的$\theta$求这一步的$Q$)
  2. M-Step : Given $Q^{(m+1)}$, solve for $\theta^{(m+1)} = \arg\max_\theta F(Q^{(m+1)}, \theta)$ (assume this is tractable). (用这一步的Q算这一步的θ)
- Initial values of $Q^{(0)}$ and $\theta^{(0)}$ are chosen randomly.
- Terminate until satisfactory (not always converge to the maximum, but guaranteed convergent).

Q实际上不参与优化,是靠猜的.

$Q^{(0)}$和$\theta^{(0)}$要随机猜. (会陷入局部最优)
一定可以收敛,但不一定收敛到最大值.
若L是凸的,则可以收敛到全局最大值.

Illustrative Example (Algorithm)

EM Algorithm for two-component Gaussian Mixture :

1. Take initial guesses for the parameters $\hat{\theta}_1 = (\hat{\mu}_1, \hat{\sigma}_1^2)$, $\hat{\theta}_2 = (\hat{\mu}_2, \hat{\sigma}_2^2)$, $\hat{c}$;
2. E-Step : $\hat{q}_i = P(Y_i = 1|Z = z_i, \hat{\theta}_1, \hat{\theta}_2) = \frac{\hat{c}\phi_{\hat{\theta}_2}(z_i)}{(1-\hat{c})\phi_{\hat{\theta}_1}(z_i) + \hat{c}\phi_{\hat{\theta}_2}(z_i)}$, for $i = 1, 2, \dots, n$;
3. M-Step : Compute the weighted means and variances :

$$\hat{\mu}_1 = \frac{\sum_{i=1}^n (1 - \hat{q}_i) z_i}{\sum_{i=1}^n (1 - \hat{q}_i)} \qquad \hat{\sigma}_1^2 = \frac{\sum_{i=1}^n (1 - \hat{q}_i)(z_i - \hat{\mu}_1)^2}{\sum_{i=1}^n (1 - \hat{q}_i)}$$

$$\hat{\mu}_2 = \frac{\sum_{i=1}^n \hat{q}_i z_i}{\sum_{i=1}^n \hat{q}_i} \qquad \hat{\sigma}_2^2 = \frac{\sum_{i=1}^n \hat{q}_i (z_i - \hat{\mu}_2)^2}{\sum_{i=1}^n \hat{q}_i}$$

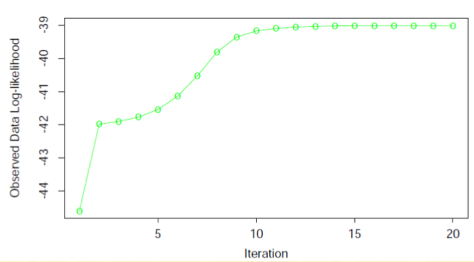
and the mixing probability $\hat{c} = \frac{1}{n} \sum_{i=1}^n \hat{q}_i$;

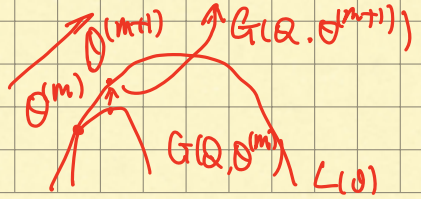
4. Iterate between E-Step and M-Step until convergence.

Illustrative Example (Result)

Iteration	1	5	10	15	20
$\hat{c}$	0.485	0.493	0.523	0.544	0.546

The final MLEs are $\hat{\mu}_1 = 4.62$, $\hat{\sigma}_1^2 = 0.87$, $\hat{\mu}_2 = 1.06$, $\hat{\sigma}_2^2 = 0.77$, $\hat{c} = 0.546$.





EM as Maximization-Maximization

- Introduce entropies as penalty to the modified objective function :

$$G(Q,\theta) = F(Q,\theta) - \sum_{i=1}^{n}\sum_{y=1}^{K} Q_{i,y}\log Q_{i,y},$$

where $Q \in \mathbb{Q} = \{Q \in [0,1]^{n,K} : \sum_{y=1}^{K} Q_{i,y} = 1, \forall i\}$

- M-Step is equivalent to : $\theta^{(m+1)} = \arg\max_{\theta} G(Q^{(m+1)},\theta)$
- E-Step is equivalent to : $Q^{(m+1)} = \arg\max_{Q\in\mathbb{Q}} G(Q,\theta^{(m)})$ (Exercise as conditional maximization) : by Jensen's inequality,

$$G(Q,\theta^{(m)}) = \sum_{i=1}^{n}\Big(\sum_{y=1}^{K} Q_{i,y}\log\frac{P_{\theta^{(m)}}(X=\mathbf{x}_i, Y=y)}{Q_{i,y}}\Big)$$
$$\leqslant \sum_{i=1}^{n}\log\Big(\sum_{y=1}^{K} Q_{i,y}\frac{P_{\theta^{(m)}}(X=\mathbf{x}_i, Y=y)}{Q_{i,y}}\Big) = L(\theta^{(m)})$$

where "=" iff $\frac{P_{\theta^{(m)}}(X=\mathbf{x}_i,Y=y)}{Q_{i,y}} = C, \forall i,y \Leftrightarrow Q_{i,y} = P_{\theta^{(m)}}(Y=y|X=\mathbf{x}_i)$.

- Monotonicity : $L(\theta^{(m+1)}) \geqslant L(\theta^{(m)})$

EM for Gaussian Mixture as Soft K-means

- For simplicity, assume $\Sigma_y = I$ for any y.
- E-Step (Partition-Step in K-Means) : $P_{\theta^{(m)}}(Y=y|X=\mathbf{x}_i) = \frac{1}{Z_i}P_{\theta^{(m)}}(Y=y)P_{\theta^{(m)}}(X=\mathbf{x}_i|Y=y) = \frac{1}{Z_i}c_y^{(m)}\exp\Big(-\frac{1}{2}\|\mathbf{x}_i-\mu_y^{(m)}\|^2\Big)$, where Z_i is a normalization factor.
- M-Step : $\max_{c_y,\mu_y}\sum_{i=1}^{n}\sum_{y=1}^{K}P_{\theta^{(m)}}(Y=y|X=\mathbf{x}_i)\Big(\log c_y - \frac{1}{2}\|\mathbf{x}_i-\mu_y\|^2\Big)$ leads to

$$\mu_y = \sum_{i=1}^{n} P_{\theta^{(m)}}(Y=y|X=\mathbf{x}_i)\mathbf{x}_i \quad \text{(Mean-Step in K-Means)}$$

$$c_y = \frac{\sum_{i=1}^{n}P_{\theta^{(m)}}(Y=y|X=\mathbf{x}_i)}{\sum_{y'=1}^{K}\sum_{i=1}^{n}P_{\theta^{(m)}}(Y=y'|X=\mathbf{x}_i)} \quad \text{(for partition in next step)}$$

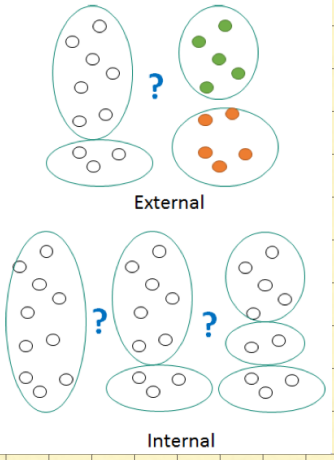
- "Soft" because the partition is done in probabilistic sense instead of deterministic sense and the average is weighted according to the probability.

Summary of EM Algorithm

- EM is unsupervised learning, an approach to perform MLE for mixture models with latent variables
- EM is an alternating optimization
- EM can be viewed as soft K-Means
- EM can deal with problems including missing data (treat missing data as latent variables and use Bayes formula, see Section 8.5.2 in the book "Elements of Statistical Learning" for general EM algorithm).
- EM can be used in the framework of Bayesian reasoning (MAP), e.g., Variational Bayesian EM algorithm
- EM is related to generative model, e.g., EM for Gaussian mixture is a population approach to learning the sample distributions, analogous to Gibbs sampling which is sampling approach to learning the distribution.
- EM is a general methodology, even used in natural language processing (e.g., latent dirichlet allocation), deep learning (e.g., restricted Boltzmann machine, deep belief network)

Model Assessment
Two Types of Indices

- External indices : validate against ground truth (labels), or compare two clusters (how similar)
  - Purity
  - Jaccard coefficient and Rand index
  - Mutual information
- Internal indices : validate without external info, based on the within-cluster similarity and between-cluster distance
  - Davies-Bouldin index (DBI)
  - Silhouette coefficient (SI)

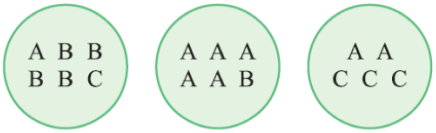


外部指标：有标签

内部指标：无标签.

Purity 纯度

- Let n_{ij} be the number of samples that belong to label j but were assigned to cluster i
- Then $n_i = \sum_{j=1}^{C}$ is the total number of samples in cluster i
- $p_{ij} = n_{ij}/n_i$ is the probability distribution in cluster i
- Purity of cluster i : $p_i \triangleq \max_j p_{ij}$
- Total purity $\triangleq \sum_i \frac{n_i}{n} p_i$
- Example : purity $= \frac{6}{17}\frac{4}{6} + \frac{6}{17}\frac{5}{6} + \frac{5}{17}\frac{3}{5} = 0.71$
- Naive case : treating each sample as a cluster leads to purity 100%



n_{ij}：本应为 j 却被分为 i.

n_i：i 中样本数

$p_{ij} = \frac{n_{ij}}{n_i}$

聚类 i 的纯度：$p_i = \max_j p_{ij}$

总纯度：$\sum_i \frac{n_i}{n} p_i$

Confusion Matrix 混淆矩阵

- SS (True Positive or TP) : # of pairs of samples belonging to the same cluster in both models
- DD (True Negative or TN) : # of pairs of samples belonging to different clusters in both models
- SD (False Positive or FP) : # of pairs of samples belonging to the same cluster in clustering model, but different clusters in reference model
- DS (False Negative or FN) : # of pairs of samples belonging to different clusters in clustering model, but the same cluster in reference model

Reference model \ Clustering model	Same Cluster	Different Cluster
Same class	SS	DS
Different class	SD	DD

以点对出现

与分类的类似.

Jaccard Coefficient and Rand Index

- Rand index (RI) : $RI = \frac{SS+DD}{SS+SD+DS+DD} \in [0,1]$, similar to the accuracy in classification problems
- Jaccard coefficient (JC) : $JC = \frac{SS}{SS+SD+DS} \in [0,1]$, compare the similarity and diversity of the samples
- Example : # of pairs in the same cluster in clustering model $= SS + SD = C_6^2 + C_6^2 + C_5^2 = 40$, and $SS = \underbrace{C_4^2}_{cluster1} + \underbrace{C_5^2}_{cluster2} + \underbrace{C_3^2 + C_2^2}_{cluster3} = 20$, so $SD = 20$; # of pairs in the same cluster in clustering model $= DS + DD = 6 \times 6 + 6 \times 5 + 6 \times 5 = 96$, and $DS = \underbrace{4 \times 1}_{B} + \underbrace{1 \times 5 + 1 \times 2 + 5 \times 2}_{A} + \underbrace{1 \times 3}_{C} = 24$, so $DD = 72$.

$$RI = \frac{20+72}{20+20+24+72} = 0.68, \quad JC = \frac{20}{20+20+24} = 0.31$$

→ 相似距离

→ 是距离

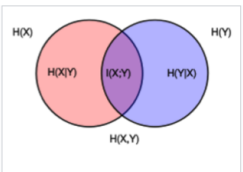
Mutual Information 互信息

- Mutual information (MI) measures the uncertainty decrement of one random variable given another random variable
- Probability that a sample belongs to both cluster u_i and v_j : $p_{UV}(i,j) = \frac{|u_i \cap v_j|}{n}$ (有标签是U 自己的是V)
- Its marginal probabilities are : $p_U(i) = \frac{u_i}{n}$ and $p_V(j) = \frac{v_j}{n}$
- Mutual information : $I(U,V) = \sum_{i=1}^{R}\sum_{j=1}^{C} p_{UV}(i,j) \log \frac{p_{UV}(i,j)}{p_U(i)p_V(j)}$
- MI attains its maximum $\min\{H(U), H(V)\}$ only when we have many small clusters
- Normalized MI : $NMI(U,V) = \frac{I(U,V)}{(H(U)+H(V))/2}$

- Entropy : $H(X) = -\sum_x p(x) \log p(x)$
- Conditional entropy :

$$H(X|Y) = \sum_y p(y) H(X|Y=y)$$
$$= \sum_y p(y)(-\sum_x p(x|y) \log p(x|y)))$$

- MI : $I(X;Y) = H(X) - H(X|Y)$
  $= H(Y) - H(Y|X)$



$$H(X,Y) = -\sum_{i=1}^{n}\sum_{j=1}^{n} p(X=x_i, Y=y_j) \log p(X=x_i, Y=y_j)$$
$$= -\sum_i \sum_j p(Y=y_j|X=x_i)p(X=x_i)[\log p(X=x_i) + \log p(Y=y_j|X=x_i)]$$
$$= -\sum_i p(X=x_i) \log p(X=x_i) \sum_j p(Y=y_j|X=x_i) - \sum_i p(X=x_i)$$
$$(\sum_j p(Y=y_j|X=x_i) \log p(Y=y_j|X=x_i))$$
$$= -\sum_i p(X=x_i) \log p(X=x_i) + H(Y|X) = H(X) + H(Y|X)$$

同理有 $H(X,Y) = H(Y) + H(X|Y)$

互信息: $I(X,Y) = H(X) + H(Y) - H(X,Y)$

Davies-Bouldin Index and Silhouette Coefficient.

- Davies-Bouldin index (DBI) measures both the within-cluster divergence and between-clusters distance
- $DBI = \frac{1}{k}\sum_{i=1}^{k} \max_{j \neq i}\left(\frac{div(c_i)+div(c_j)}{d(\mu_i,\mu_j)}\right)$ where $div(c_i)$ represents the average distance of samples within cluster c_i, μ_i is the center of cluster c_i
- Silhouette Coefficient (SC) : $SC = \frac{b_i - a_i}{\max(a_i,b_i)}$, where a_i is (第i个样本到同聚类中其他样本的平均距离) average distance between the i-th sample and every other sample in the same cluster, b_i is the minimal distance from the i-th sample to the other clusters; range is $[-1,1]$ (第i个样本到其他聚类的最近距离)
- The smaller the DBI, or the larger the SC, the better the clustering results

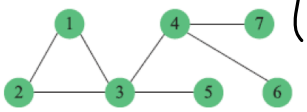
div(ci) 类内的散度 = 可用距离平均替代.

DBI越小越好. SC越大越好.

Spectral Clustering 谱聚类

Graphs

- A set of data points $\{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$, similarity s_{ij} or distance d_{ij}
- Graph $G = (V, E)$, where $V = \{v_i\}_{i=1}^n$ with each v_i representing a sample $\mathbf{x}_i$
- v_i and v_j are connected ($w_{ij} > 0$) if $s_{ij} > \epsilon$ where $\epsilon \geqslant 0$ is a threshold; then the edge is weighted by $w_{ij} = s_{ij}$
- Undirected graph $w_{ij} = w_{ji}$, adjacency matrix $W = \{w_{ij}\}$
- Degree of v_i : $d_i = \sum_{j=1}^n w_{ij}$; $D = \mathrm{diag}(d_1, \ldots, d_n)$



$$D = \begin{bmatrix} 2 & & & & & & \\ & 2 & & & & & \\ & & 4 & & & & \\ & & & 3 & & & \\ & & & & 1 & & \\ & & & & & 1 & \\ & & & & & & \end{bmatrix}$$

$$W = \begin{bmatrix} 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \end{bmatrix}$$

D表示节点i与多少个其他节点相连，是对角矩阵。

Similarity Graphs

- ϵ-neighborhood graph : v_i and v_j are connected if $d(x_i, x_j) < \epsilon$; unweighted graph; $\epsilon \sim (\log n/n)^p$; difficult to choose ϵ for data on different scales
- k-nearest neighbor graph : connect v_i to v_j if v_j is among the k-nearest neighbors of v_i, directed graph; connect v_i and v_j if v_i and v_j are among the k-nearest neighbors of each other, mutual k-nearest neighbor graph, undirected; $k \sim \log n$
- Fully connected graph : connect all points with positive similarity with each other; model local neighborhood relationships; Gaussian similarity function $s(x_i, x_j) = \exp(-\|x_i - x_j\|^2/(2\sigma^2))$, where σ controls the width of neighborhoods; adjacency matrix is not sparse; $\sigma \sim \epsilon$

ε近邻图
算ε前一般先对数据归一化。

k近邻图

全连接图
全部节点都连起来，且权重为
$$W_{ij} = \begin{cases} e^{\frac{-\|x_i - x_j\|_2^2}{2\sigma^2}}, & i \neq j \\ 0, & i = j \end{cases}$$
σ越大，聚类范围越大。

Graph Laplacian 图拉普拉斯

- Unnormalized graph Laplacian : $L = D - W$
  - Has $\mathbf{1}$ as an eigenvector corresponding to the eigenvalue 0
  - Symmetric and positive (semi) definite : $\mathbf{f}^T\mathbf{L}\mathbf{f} = \frac{1}{2}\sum_{i,j} w_{ij}(f_i - f_j)^2 \geqslant 0$
  - Non-negative, real-valued eigenvalues $0 = \lambda_1 \leqslant \lambda_2 \leqslant \cdots \leqslant \lambda_n$
  - The eigenspace of eigenvalue 0 is spanned by the indicator vectors $\mathbf{1}_{A_1}, \ldots, \mathbf{1}_{A_k}$, where $A_1, \ldots, A_k$ are k connected components in the graph
- Normalized graph Laplacians :
  - Symmetric Laplacian : $L_{sym} = D^{-1/2}LD^{-1/2}$
  - Random walk Laplacian : $L_{rw} = D^{-1}L$
  - Both have similar properties as L

必有一个为0的特征值，且该特征值的特征向量为$\vec{1}$.

$$L\vec{1} = D\begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix} - W\begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix} = \begin{pmatrix} d_1 \\ \vdots \\ d_n \end{pmatrix} - \begin{pmatrix} \sum_{j=1}^n w_{1j} \\ \vdots \\ \sum_{j=1}^n w_{nj} \end{pmatrix} = 0$$

是对称半正定的。 因为 $d_i = \sum_{j=1}^n w_{ij}$.

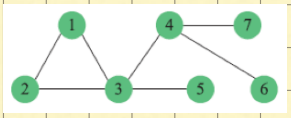
$$f^TLf = f^TDf - f^TWf = \sum_i d_i f_i^2 - \sum_{i,j} w_{ij} f_i f_j$$

$$= \sum_i \underbrace{\left(\sum_j w_{ij}\right)}_{d_i} f_i^2 - \sum_{i,j} w_{ij} f_i f_j = \frac{1}{2}\sum_{i,j} w_{ij}(f_i - f_j)^2 \geqslant 0$$

$x^TAx = \sum a_{ij}x_ix_j$

所有特征值是非负的实数
特征值0对应的特征向量可能不止一个.
(有几个连通分支，0特征值就有几个特征向量)

Random walk Laplacian 中除对角线上的元素，其绝对值取值在[0,1]之间，且同行绝对值和为1.



$$L = \begin{pmatrix} 1 & -\frac{1}{2} & -\frac{1}{2} & 0 & 0 & 0 & 0 \\ -\frac{1}{2} & 1 & -\frac{1}{2} & 0 & 0 & 0 & 0 \\ -\frac{1}{4} & -\frac{1}{4} & 1 & -\frac{1}{4} & -\frac{1}{4} & 0 & 0 \\ 0 & 0 & -\frac{1}{3} & 1 & 0 & -\frac{1}{3} & -\frac{1}{3} \\ 0 & 0 & -1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 1 \end{pmatrix}$$

从某个节点到另一个节点都可看作一个概率值.

$$P(a \xrightarrow{k\text{-step}} b) = (D^{-1}W)^k_{a,b}$$

从节点a经k步到节点b

$$D^{-1}L = I - D^{-1}W$$

Spectual Clustering

- Graph cut : segment G into K clusters $A_1, \dots, A_K$, where $A_i \subset V$, this is equivalent to minimize the graph cut function

$$cut(A_1, \dots, A_K) = \frac{1}{2} \sum_{k=1}^{K} W(A_k, \bar{A}_k)$$

where $W(A, B) = \sum_{i \in A, j \in B} w_{ij}$. Trivial solution consists of a singleton and its complement

- RatioCut : $RatioCut(A_1, \dots, A_K) = \frac{1}{2} \sum_{k=1}^{K} \frac{W(A_k, \bar{A}_k)}{|A_k|}$, where $|A|$ is the number of vertices in A
- Normalized cut : $Ncut(A_1, \dots, A_K) = \frac{1}{2} \sum_{k=1}^{K} \frac{W(A_k, \bar{A}_k)}{vol(A_k)}$, where $vol(A) = \sum_{i \in A} d_i$; it is NP-hard

将分割的权值和最小.

限制子图的大小.

用度表示子图大小

NP-hard

Relaxation of RatioCut to Eigenvalue Problems with K=2.

- $\min_{A \subset V} RatioCut(A, \bar{A})$
- Binary vector $f = (f_1, \dots, f_n)^T$ as indicator function : $f_i = \begin{cases} \sqrt{|\bar{A}|/|A|}, & \text{if } v_i \in A \\ -\sqrt{|A|/|\bar{A}|}, & \text{if } v_i \in \bar{A} \end{cases}$
- $f^T L f = |V| \cdot RatioCut(A, \bar{A})$, $\sum_{i=1}^{n} f_i = 0$, and $\|f\|_2^2 = n$
- Relax f to be real-valued : $\min_{f \in \mathbb{R}^n} f^T L f$, subject to $f \perp \mathbf{1}$ and $\|f\|_2 = \sqrt{n}$
- By Rayleigh-Ritz theorem, the solution f is the eigenvector corresponding to the second smallest eigenvalue of L
- Cluster $\{f_i\}_{i=1}^n$ to two groups C and $\bar{C}$: $v_i \in A$ if $f_i \in C$, and else $v_i \in \bar{A}$

$$f^T L f = \frac{1}{2} \sum_{ij} w_{ij} (f_i - f_j)^2$$

$$= \sum_{\substack{i \in A \\ j \notin A}} w_{ij} \left(\sqrt{\frac{|\bar{A}|}{|A|}} + \sqrt{\frac{|A|}{|\bar{A}|}} \right)^2$$

$$= \sum_{\substack{i \in A \\ j \notin A}} w_{ij} \left(\frac{n^2}{|A||\bar{A}|} \right) = n \, RatioCut(A, \bar{A})$$

$\min_{f \in \{\text{indicator}\}} f^T L f$ 仍是一个 NP-hard 问题. 将 f 范围扩大,

$\Downarrow$

$\min_{f \in \mathbb{R}^n} f^T L f$, 转成特征值问题

Relaxation of RatioCut and NCut with general K.

- RatioCut
  - Binary vector $h_j = (h_{1j}, \dots, h_{nj})^T$, $j = 1, \dots, K$, as indicator function : $h_{ij} = \begin{cases} 1/\sqrt{|A_j|}, & \text{if } v_i \in A_j \\ 0, & \text{otherwise} \end{cases}$ h_j代表A_j的示性函数
  - $h_j^T L h_j = Cut(A_j, \bar{A}_j)/|A_j|$, $H = (h_1, \dots, h_K) \in \mathbb{R}^{n \times K}$, $RatioCut(A_1, \dots, A_K) = \mathrm{Tr}(H^T L H)$, $H^T H = I$
  - Relax H : $\min_{H \in \mathbb{R}^{n \times K}} \mathrm{Tr}(H^T L H)$, subject to $H^T H = I$ (扩大)
  - Solution : the first K eigenvectors of L as columns
  - Cluster the rows of H to K groups
- Ncut
  - Replacing $|A_j|$ by $vol(A_j)$, the same argument for the relaxation of Ncut : $\min_{H \in \mathbb{R}^{n \times K}} \mathrm{Tr}(H^T L H)$, subject to $H^T D H = I$ (实际上是对 $D^{-1}L$ 的特征分解)
  - Solution : the first K eigenvectors of L_{rw} as columns

$$h_j^T h_j = 1$$

$$\sum_{i=1}^{n} h_{ij}^2 = \sum_{i \in A_j} \frac{1}{|A_j|} = 1$$

$$h_j^T h_k = \sum_{\substack{i \in A_j \\ i \notin A_k}} h_{ij} h_{ik} = 0 \quad (j \neq k)$$

$A_j \cap A_k = \phi$

$$H^T L H = \begin{pmatrix} h_1^T \\ \vdots \\ h_K^T \end{pmatrix} L (h_1 \dots h_K) = \begin{pmatrix} h_1^T L h_1 & h_1^T L h_2 & \cdots \\ h_2^T L h_1 & \ddots & \\ \vdots & & \end{pmatrix}$$

$$\mathrm{tr}(H^T L H) = \sum_{i=1}^{K} h_i^T L h_j = RatioCut(A_1, \dots, A_K)$$

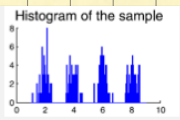
L 的每一行看作一个样本. 一共 n 个样本分成 K 组.

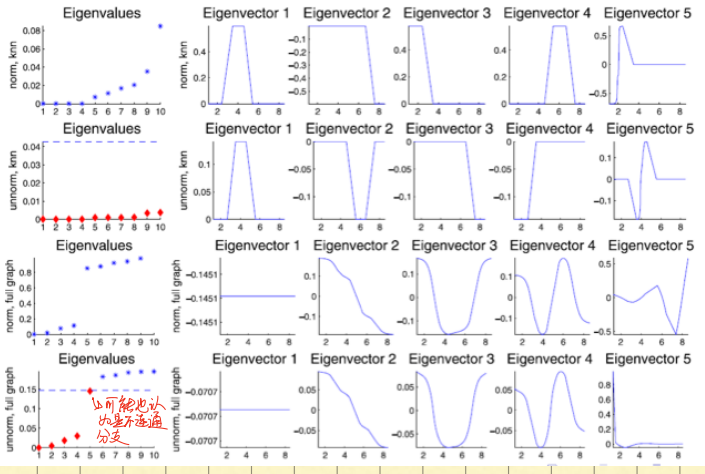
(用 K-means)

Spectual Clustering Algorithm

- Input : Similarity matrix $S \in \mathbb{R}^{n \times n}$, number k of clusters
- Output : Clusters $A_1, \ldots, A_K$ of indices of vertices
- Algorithm :
  1. Construct a similarity graph $G = (V, E)$ with weighted adjacency matrix W
  2. Compute the unnormalized graph Laplacian L or normalized graph Laplacian L_{sym} or L_{rw}
  3. Compute the first K eigenvectors $\mathbf{U} = [\mathbf{u}_1, \ldots, \mathbf{u}_K] \in \mathbb{R}^{n \times K}$
  4. In the case of L_{sym}, normalize the rows of U to norm 1 ; for the other two cases, skip this step
  5. Let $\mathbf{y}_i \in \mathbb{R}^K$ be the i-th row of $\mathbf{U}$, use K-means to cluster the point set $\{\mathbf{y}_i\}_{i=1}^n$ into clusters $C_1, \ldots, C_K$
  6. $A_k = \{i | y_i \in C_k\}$

Mixture of 4 Gaussians on $\mathbb{R}$:



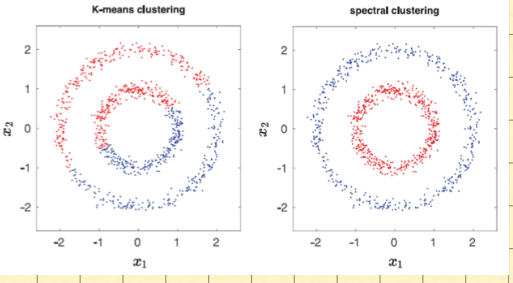


K近邻图
归一化和未归一化不一样
用谱聚类建议归一化

全连接图

Interpretations

- Usually better than K-means



显然谱聚类优于 K-means

Random Walks Point of View

- $P = D^{-1}W$ can be interpreted as transition matrix of a Markovian random walk, which possesses a unique stationary distribution if the graph is connected and non-bipartite.
- $L_{rw} = I - P \Rightarrow \lambda(L_{rw}) = 1 - \lambda(P)$
- A probability viewpoint of Ncut : for a random walk $(X_t)_t$ starting with X_0 in the stationary distribution,

$$Ncut(A, \bar{A}) = P(X_1 \in \bar{A} | X_0 \in A) + P(X_1 \in A | X_0 \in \bar{A}).$$

  Minimizer of Ncut gives a segmentation of the graph such that a random walk seldom transitions between A and $\bar{A}$
- Commute distance : c_{ij} measures the expected time it takes the random walk to travel from vertex i to vertex j and back. Some better properties than shortest path (geodesics). A nice formula :

$$c_{ij} = vol(V)(e_i - e_j)^T L^{\dagger}(e_i - e_j)$$

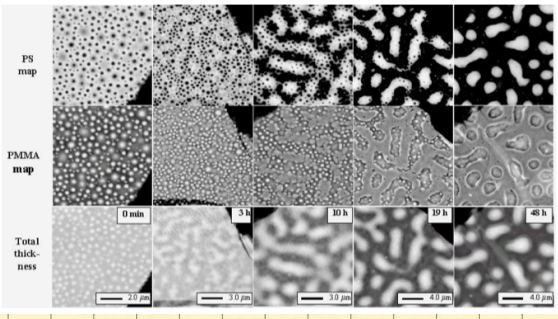
  where $L^{\dagger}$ is psudo-inverse of L.

Ginzburg-Landau Segmentation

- Ginzburg-Landau functional :

$$GL(u) = \frac{\epsilon}{2} \int |\nabla u|^2 \mathrm{d}x + \frac{1}{\epsilon} \int W(u) \mathrm{d}x,$$

  where $W(u) = \frac{1}{4}(u^2 - 1)^2$ is a double well potential. This is used to model superconductivity, two-phase flows, etc. The minimizer naturally separates the "+1" phase from the "-1" phase.



Ginzburg-Landau Gradient Flow

- Gamma convergence : $GL(u) \rightarrow_{\Gamma} C|u|_{TV}$, widely used in image segmentation.
- Minimizing $E(u) = GL(u) + \lambda F(u, u_0)$ (F is data fidelity) is usually driven by a gradient flow :

$$u_t = \epsilon \Delta u - \frac{1}{\epsilon} W'(u) - \lambda \frac{\delta F}{\delta u}.$$

- Numerical PDE solver by convex splitting of $E(u) = E_{convex} - E_{concave}$:

$$\frac{u^{n+1} - u^n}{\Delta t} = -\frac{\delta E_{convex}}{\delta u}(u^{n+1}) + \frac{\delta E_{concave}}{\delta u}(u^n)$$

- Due to the Laplace operator (diagonalizable by Fourier transform), this can be solved very efficiently using FFT and iterated in spectral space

Ginzburg-Landau Segmentation on Graphs

- Bertozzi and Flenner introduced modified GL functional on graph $G = (V, E)$:

$$E(u) = \frac{\epsilon}{2} < u, Lu > + \frac{1}{4\epsilon} \sum_{z \in V} (u^2(z) - 1)^2 + \sum_{z \in V} \frac{\lambda(z)}{2} (u(z) - u_0(z))^2,$$

where u is the labeling function

Convex Splitting for the Graph Laplacian

1. Input $\leftarrow$ an initial function u_0 and the eigenvalue-eigenvector pairs $(\lambda_k, \phi_k(x))$ for the graph Laplacian L_s from (2.6).
2. Set convexity parameter c and interface scale ϵ from (3.2).
3. Set the time step dt.
4. Initialize $a_k^{(0)} = \int u(x)\phi_k(x)\, dx$.
5. Initialize $b_k^{(0)} = \int [u_0(x)]^3 \phi_k(x)\, dx$.
6. Initialize $d_k^{(0)} = 0$.
7. Calculate $\mathcal{D}_k = 1 + dt\,(\epsilon\, \tilde{\lambda}_k + c)$.
8. For n less than a set number of iterations M
   (a) $a_k^{(n+1)} = \mathcal{D}_k^{-1} \left[\left(1 + \frac{dt}{\epsilon} + c\, dt\right) a_k^{(n)} - \frac{dt}{\epsilon} b_k^{(n)} - dt d_k^{(n)} \right]$,
   (b) $u^{(n+1)}(x) = \sum_k a_k^{(n+1)} \phi_k(x)$,
   (c) $b_k^{(n+1)} = \int [u^{(n+1)}(x)]^3 \phi_k(x)\, dx$,
   (d) $d_k^{(n+1)} = \int \lambda(x)\, (u^{(n+1)}(x) - u_0(x))\, \phi_k(x)\, dx$.
9. end for
10. Output $\leftarrow$ the function $u^{(M)}(x)$.

Ginzburg-Landau Segmentation on Two-moon Data

$\epsilon = 10$ $\epsilon = 2.6$ $\epsilon = 2$