STAT 542: Statistical Learning

Clustering

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Course Website: https://teazrq.github.io/stat542/

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Unsupervised Learning

Unsupervised Learning

- No response variable Y, only $\{x_i\}_{i=1}^n$.
- Goal: learn patterns in X.
- Examples
  - Estimate the density, covariance, graph (network), etc. of X — could be difficult in high-dimensional settings
  - Cluster analysis: identify multiple regions of the feature space that contains modes of density.
  - Dimension reduction: identify low-dimensional manifold within the feature space $\mathcal{X}$ that represents high data density.
- Oftentimes, there is no clear measure of success.

Cluster Analysis

Cluster Analysis

- Group the dataset into subsets so that those within each subset are more closely related (similar) to each other than those objects assigned to other subsets. Each subset is called a cluster
- Flat clustering vs. hierarchical clustering: flat clustering divides the dataset into k cluster, and hierarchical clustering arranges the clusters into a natural hierarchy.
- Clustering results are crucially dependent on the measure of similarity (or distance) between the “points” to be clustered.

Distance Metric

- A distance metric or a distance function is a function that defines the similarity of two elements (points, sets, etc.)
- For the distance of two points (with continuous entries), the most commonly used measurement is the Euclidian distance:

$$\begin{aligned} d(u, v) &= \|u - v\|_2 \\ &= \sqrt{\textstyle\sum_{j=1}^{p} (u_j - v_j)^2} \end{aligned}$$

- For categorical entries, the Hamming distance is usually used

$$d(u, v) = \textstyle\sum_{j=1}^{p} \mathbf{1}\{u_j \neq v_j\}$$

- Distance measures should be defined based on the application. There is no universally best approach.

Clustering

- Suppose we have a set of n data points
- We want to form $K \ll n$ clusters, indexed by $k \in \{1, \dots, K\}$.
- Let $C(\cdot)$ be a cluster index function that assign th ith observation or cluster $C(i)$.
- Consider: search for a function $C : \{1, \dots, n\} \to \{1, \dots, K\}$ to minimize the within cluster distance:

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

Clustering

- This is equivalent to maximizing the between cluster distance

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

- Note that the total distance can be broke down into

$$T = \frac{1}{2} \sum_{i=1}^{n} \sum_{i'=1}^{n} d_{ii'} = \frac{1}{2} \sum_{k=1}^{K} \sum_{C(i)=k} \left[\sum_{C(i')=k} d_{ii'} + \sum_{C(i')\neq k} d_{ii'} \right]$$
$$= W(C) + B(C)$$

- The total distance is fixed for a given set of data, hence

$$\text{minimize } W(C) \iff \text{ maximize } B(C)$$

Clustering

- Given a specific distance measure $d(\cdot, \cdot)$, several algorithms can be used to find the clusters
  - Combinatorial algorithm
  - K-means clustering
  - Hierarchical clustering

Combinatorial Algorithm

Combinatorial Algorithms

- For small n and K, we could minimize W by brute-force search.
- However, the number of “tries” needed to complete the search is

$$S(n, K) = \frac{1}{K!}\sum_{k=1}^{K}(-1)^{K-k}\binom{K}{k}k^n$$

- For example $S(10, 4) = 34, 105$; $S(19, 4) \approx 10^{10}$.
- This is not feasible for large n and K, since the number of distinct assignments can be extremely large.
- It calls for more efficient algorithms: may not be optimal but a reasonably good suboptimal partition.

K-means Clustering

K-means Clustering

- Consider an enlarged optimization problem:

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

- Hence, we are solving both
    - the cluster index function $C(\cdot)$,
    - and also the cluster centers m_k, $k = 1 \dots K$.
- This problem is NP-hard for ≥ 2 dimensions.

K-means Clustering

- Combinatorial algorithm is too expansive.
- Instead, consider an algorithm that alternatively updates the two components:
  - C, the cluster assignments
  - $\{m_k\}_{k=1}^K$: the cluster means
- We will do an iterative update by:
  1) Fixing C, find the best $\{m_k\}_{k=1}^K$
  2) Fixing $\{m_k\}_{k=1}^K$, find the best C

K-means Clustering

- Fixing C, we know the cluster label of each subject. For any set $\{i : C(i) = k\}$, finding the mean is

$$m_k = \arg\min_m \sum_{C(i)=k} \|x_i - m\|^2.$$

- This is simply finding the mean within cluster k, i.e.

$$m_k = \frac{\sum_{C(i)=k} x_i}{\sum_i \mathbf{1}\{C(i) = k\}}$$

K-means Clustering

- Fixing the cluster means $\{m_k\}_{k=1}^{K}$, to find the new cluster assignments, we simply recalculate the distance from an observation to each of the cluster mean.

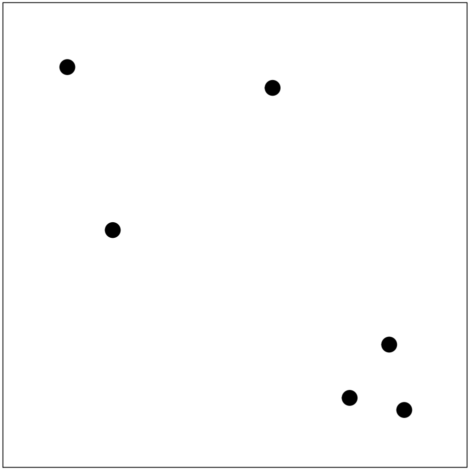
$$C(i) = \underset{k \in \{1,\ldots,K\}}{\arg\min} \quad d(x_i, m_k)$$

- Hence each point will be assigned to the closest cluster mean

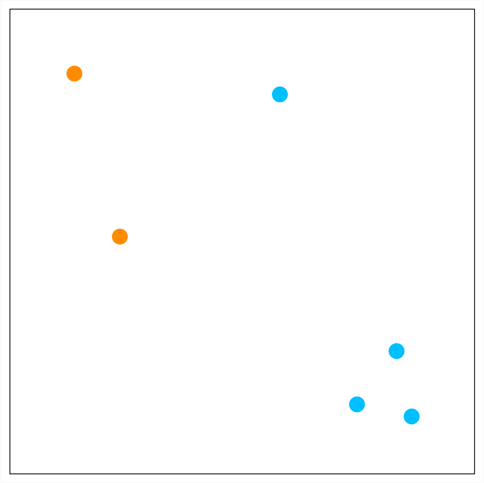
K-means Clustering

- A K-means Clustering algorithm:
    1) Randomly split the dataset into K different subsets. Assign each subsets a cluster label. Then iterate between 2) and 3).
    2) Given the cluster assignment C, calculate the cluster mean vectors $m_1, \ldots, m_K$.
    3) Given the current set of means $\{m_1, \ldots, m_K\}$, assign each observation to the closest current cluster mean.
- Stop the algorithm when C does not change

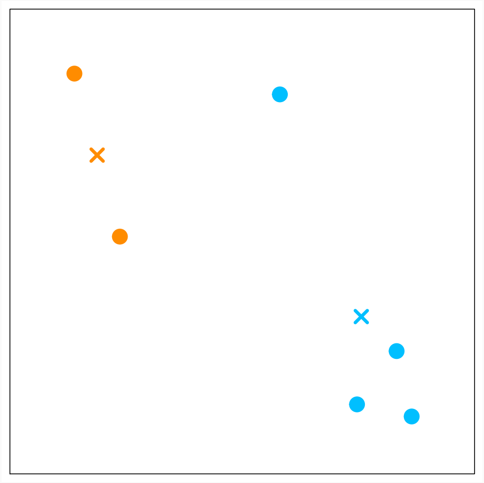
Demonstration



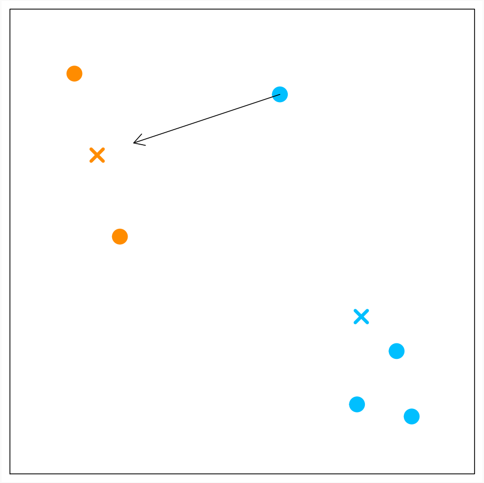
Demonstration



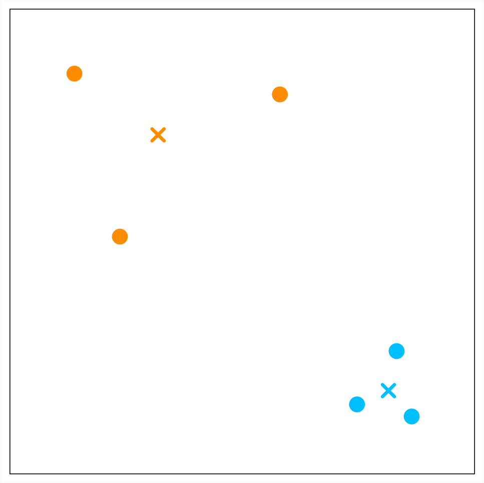
Demonstration



Demonstration



Demonstration



K-means Clustering

- Note: We usually initiate the cluster labels randomly. However, this algorithm does not guarantee to global minimum. Example?
- The algorithm still has a descent property, which leads to a local minimizer.

Alternative Version

- K-medoids is an alternative version of K-means:
- Replace the second step by searching for the one observation that minimizes the distance to all others in the cluster

$$i_k^* = \underset{i:C(i)=k}{\arg\min} \sum_{C(i')=k} D(x_i, x_{i'})$$

- Use $x_{i_k^*}$ as the "center" of cluster k.

Applications

- See the supplementary R file
- Example 1: the iris data
- Example 2: cluster pixels in a picture

Remarks

- Clustering may help in supervised learning
- How to choose the number of clusters K
- Other distance measures
- Categorical variables

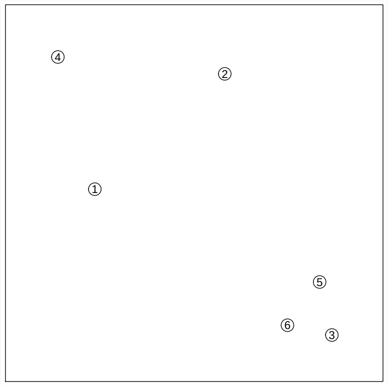
Hierarchical Clustering

Hierarchical Clustering

- Choosing the number of clusters K can be difficult
- A hierarchical representation which
  - at the lowest level, each cluster contains a single observation.
  - at the highest level there is only one cluster containing all observations.
- Use dendrogram to display the clustering result.

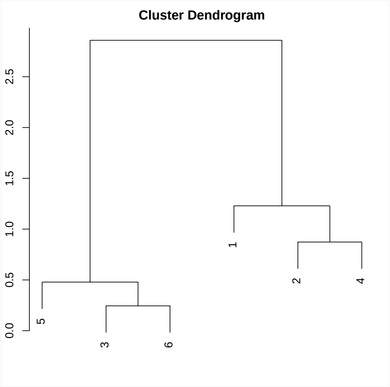
Hierarchical Clustering

- Suppose we have a set of 6 observations

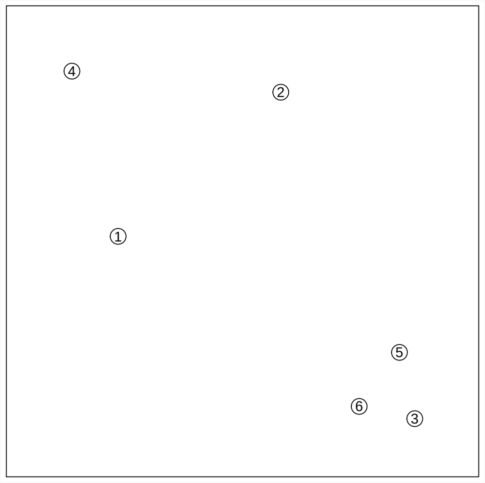


Dendrogram

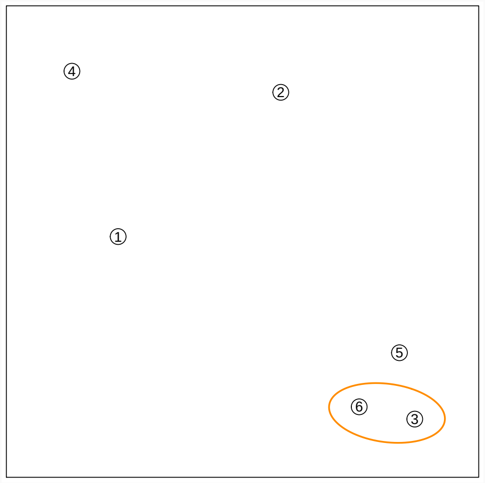
- A typical dendrogram from hierarchical clustering
- How to construct this?



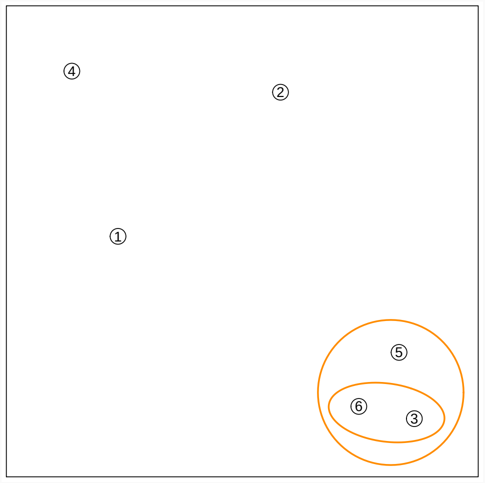
Demonstration



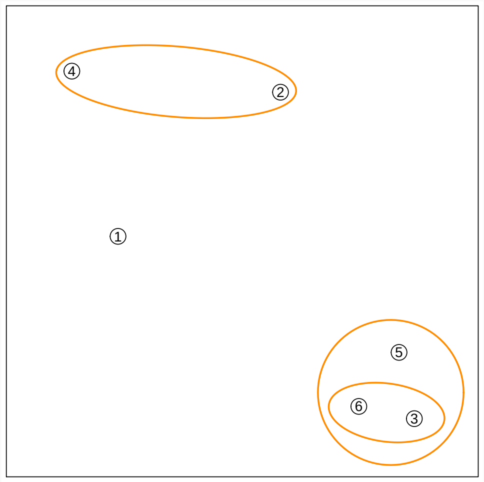
Demonstration



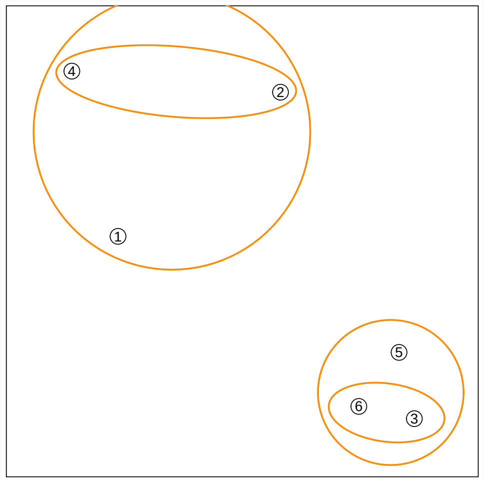
Demonstration



Demonstration



Demonstration



Algorithm (agglomerative)

- An agglomerative algorithm is a “bottom up” approach:
  - Begin with every observation representing a singleton cluster.
  - At each step, merge two “closest” clusters into one cluster and reduce the number of clusters by one.
  - Stop when all observations are in the same cluster
- How to choose which two clusters to merge?
- This requires:
  - A distance measure between any two observations $d(x_i, x_{j'})$
  - A distance measure between any two sets of observations $d(G, H)$

Distance Measures

- Distance $d(G, H)$ between two clusters G and H can be defined in different ways:
  - Complete linkage (default of hclust()): the furthest pair

$$d(G, H) = \max_{i \in G, i' \in H} d_{ii'}$$

  - Single linkage: the closest pair

$$d(G, H) = \min_{i \in G, i' \in H} d_{ii'}$$

  - Average linkage: average dissimilarity

$$d(G, H) = \frac{1}{n_G n_H} \sum_{i \in G} \sum_{i' \in H} d_{ii'}$$

- Different choice may results in different hierarchical structures

Distance Matrix

- To perform a hierarchical clustering, a matrix of all the pair-wise distances is sufficient
- We don't have to know the values of the original observations
- This is an $n \times n$ matrix: the (i, i')'s element represents the distance between x_i and $x_{i'}$
- This matrix is also called a dissimilarity matrix.
    - Symmetric
    - diagonal elements are zero

Applications

- See the supplementary R file
- Example 1: the iris data
- Example 2: RNA expression data

Principle Component Analysis

Principle Component Analysis

- Principle Component Analysis (PCA) is an old but very useful technique invented by Karl Pearson in 1901
- The main purpose is data visualization (mostly in 2d)
- It also serves as a dimension reduction method
- Unsupervised method, can be used for preprocessing the data.

Principle Component Analysis

- Given that we have a $n \times p$ design matrix $\mathbf{X}$, there are many equivalent approaches (motivations):
  - Explain the most variation: Produce a derived set of uncorrelated variables $\mathbf{Z}_k = \mathbf{X}\alpha_k$, $k = 1, \ldots, q < p$ that are linear combinations of the original variables, and explain most of the variation in the original set
  - Approximate the design matrix: Approximate the design matrix $\mathbf{X}$ by the best (using Frobenius norm) rank-q matrix, which can be performed through SVD

Principle Component Analysis

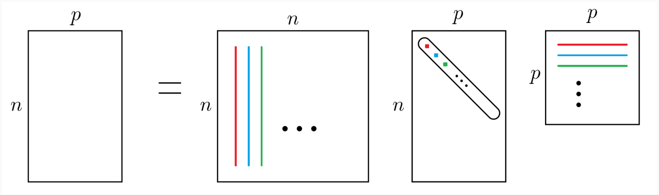
- Suppose we have an $n \times p$ design matrix $\mathbf{X}$
- The first step is to center each variable, i.e., subtract the column means from each column respectively.
- In the following, we assume that $\mathbf{X}$ is already centered.
- Centering $\mathbf{X}$ does nothing but re-positioning the axis

Singular Value Decomposition

- One way to understand the PCA is using a singular value decomposition (SVD)

$$\mathbf{X}_{n\times p} = \mathbf{U}_{n\times n}\mathbf{D}_{n\times p}\mathbf{V}^{\mathsf{T}}_{p\times p},$$

where both $\mathbf{U}$ and $\mathbf{V}$ are orthogonal matrices, i.e. $\mathbf{U}^{\mathsf{T}}\mathbf{U} = \mathbf{U}\mathbf{U}^{\mathsf{T}} = \mathbf{I}$, and same for $\mathbf{V}$; and $\mathbf{D}_{n\times p}$ is a diagonal matrix.



- The diagonal elements of $\mathbf{D}_{n\times p}$ are of a decreasing order.

Low Rank Approximation

- If we have to choose a rank-1 matrix $\mathbf{A}$ to approximate $\mathbf{X}_{n\times p}$, what would we do?
- Turns out that the best choice is

$$\mathbf{U}_1 d_{11} \mathbf{V}_1^\mathsf{T},$$

  where $\mathbf{U}_1$ is the first column of $\mathbf{U}$, $\mathbf{V}_1$ is the first column of $\mathbf{V}$, and d_{11} is the first diagonal element of $\mathbf{D}$
- In other words, $\|\mathbf{X} - \mathbf{U}_1 d_{11} \mathbf{V}_1^\mathsf{T}\|_2^2$ is minimized with this choice.
- Hence, $\mathbf{U}_1 d_{11} \mathbf{V}_1^\mathsf{T}$ is a rank-1 matrix that explained the variations in $\mathbf{X}$ as much as possible.

Principle Component Analysis

- Let's consider the sample covariance matrix $\widehat{\Sigma} = \mathbf{X}^\mathsf{T}\mathbf{X}/(n-1)$, since $\mathbf{X}$ is already centered.
- $\widehat{\Sigma}$ can be diagonalize into

$$\widehat{\Sigma} = \mathbf{V}\mathbf{D}^*\mathbf{V}^\mathsf{T},$$

  where columns of $\mathbf{V}$ are principle directions (loadings) and projecting $\mathbf{X}$ on these loadings gives the principal components
- On the other hand, based on SVD,

$$\mathbf{X} = \mathbf{U}\mathbf{D}\mathbf{V}^\mathsf{T},$$

  we can rewrite $\widehat{\Sigma}$ as

$$\widehat{\Sigma} = \mathbf{V}\mathbf{D}^\mathsf{T}\mathbf{U}^\mathsf{T}\mathbf{U}\mathbf{D}\mathbf{V}^\mathsf{T}/(n-1) = \mathbf{V}\frac{\mathbf{D}^2}{n-1}\mathbf{V}^\mathsf{T}$$

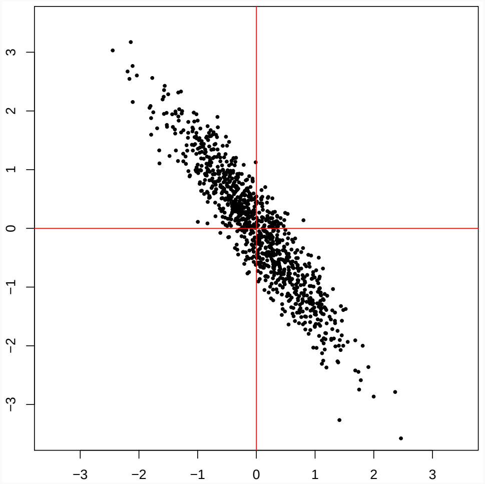
Principle Component Analysis

- So the right singular vectors $\mathbf{V}$ of $\mathbf{X}$ are just the principle directions, and the principal components are basically projecting each row (observation) of $\mathbf{X}$ onto those directions:

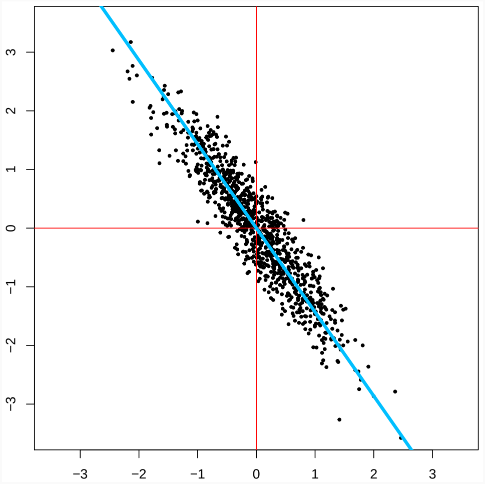
$$\mathbf{X}\mathbf{V} = \mathbf{U}\mathbf{D}\mathbf{V}^\mathsf{T}\mathbf{V} = \mathbf{U}\mathbf{D}$$

- The first column of $\mathbf{U}$ is the first PC, and d_{11} is the variation along that direction, which is also the squared eigenvalue from SVD.
- PCA should be performed by centering $\mathbf{X}$ first (column-wise, i.e., by each variable).

Demonstration



Demonstration



Principle Component Analysis

- PCA is a dimension reduction tool, often used for visualization
- The leading PCs may display interesting information of the underlying (unobserved) clusters/manifold
- PCA is unsupervised, i.e., the directions does not necessarily reflect the relationship with the response (if there is any)

Self-organizing Maps

Overview

- Self-organizing Map (SOM) is another popular clustering method
- The main difference between SOM and k-means is that cluster means of a SOM has geometric relationship
- We will introduce the algorithm
- Please see R examples from course website

SOM Algorithm

- Input data: $\{x_i\}_{i=1}^n$.
- Initialize cluster means (randomly): $w_{ij}, i = 1, \dots p, j = 1, \dots q$. are a grid of centers (the connected black dots). They are similar to the centers in a k-mean algorithm. However, they also preserves some geometric relationship.
- Learning rate: $\alpha \in [0, 1]$. This controls how fast the w_{ij}'s are updated. It will decrease progressively.
- Radius: r that controls how many w_{ij}'s will be updated at each iteration. It will also decrease progressively.

SOM Algorithm

- For $k = 1, \ldots, n$, we will steam-in one new observation x_k and perform the following update:
  - For all w_{ij}, calculate the distance between each w_{ij} and x_k. Let $d_{ij} = \|x_k - w_{ij}\|$. By default, we use Euclidean distance.
  - Select the closest w_{ij}, denoted as w_*
  - Update each w_{ij} based on the fomular $w_{ij} = w_{ij} + \alpha\, h(w_*, w_{ij}, r)\, \|x_k - w_{ij}\|$
  - Decrease the value of α and r
- In the ‘kohonen‘ package, α starts at 0.05, and linearly decreases to 0.01, while r is chosen to be 2/3 of all cluster means at the first iteration.

Spectral Clustering

Similarity Graph

- In some applications, we do not have the value of each data point, instead, we have the similarities between data points.
- Note: for similarity measures, larger means more similar, while for distance measures, larger is further away.
- A nice way to represent the data is the Similarity Graph $G = (V, E)$ — an undirected graph
    - V is a set of vertices: $\{x_1, x_2, \ldots, x_n\}$
    - E is the set of edges: $\{(i, j)\}_{ij}$

Similarity Graph

- For our case, this graph is weighted by an adjacency matrix

$$\mathbf{W}_{n\times n} = \{w_{ij}\}_{ij}$$

  - You can define $\mathbf{W}$ in many different ways
  - Each w_{ij} is the similarity between vertices i and j
  - $\mathbf{W}$ is symmetric: $w_{ij} = w_{ji}$

- We also define the degree matrix $\mathbf{D}$ as a diagonal matrix

$$\text{diag}(d_1, \ldots, d_n)$$

where the d_i is the degree of vertex i:

$$d_i = \sum_{j=1}^{n} w_{ij}$$

Graph Laplacian

- There are many different ways to define a graph Laplacian matrix. We give a few examples.
- Unnormalized graph Laplacian

$$\mathbf{L} = \mathbf{D} - \mathbf{W}$$

- Normalized graph Laplacians

$$\begin{aligned} \mathbf{L}_{\text{sym}} &= \mathbf{D}^{-1/2}\mathbf{L}\mathbf{D}^{-1/2} = \mathbf{I} - \mathbf{D}^{-1/2}\mathbf{W}\mathbf{D}^{-1/2} \\ \mathbf{L}_{\text{rw}} &= \mathbf{D}^{-1}\mathbf{L} = \mathbf{I} - \mathbf{D}^{-1}\mathbf{W} \end{aligned}$$

- Each of them have some unique properties.

Unnormalized graph Laplacian

- For the Unnormalized graph Laplacian, we have, for any f

$$
\begin{aligned}
f'\mathbf{L}f = f'\mathbf{D}f - f'\mathbf{W}f &= \sum_{i=1}^{n} d_i f_i^2 - \sum_{i,j} f_i f_j w_{ij} \\
&= \frac{1}{2}\left\{ \sum_i d_i f_i^2 - 2\sum_{i,j} f_i f_j w_{ij} + \sum_j d_j f_j^2 \right\} \\
&= \frac{1}{2}\sum_{ij} w_{ij}(f_i - f_j)^2
\end{aligned}
$$

- We also have:
    - $\mathbf{L}$ is positive semi-definite
    - the smallest eigen-value is 0, with eigen-vector $\mathbf{1}$
    - The number of 0 eigen-values depends on the number of connected components

Normalized graph Laplacian

- For the normaized graph Laplacian, we have,

$$f'\mathbf{L}_{\mathsf{sym}}f = \frac{1}{2}\sum_{ij} w_{ij}\left(\frac{f_i}{\sqrt{d_i}} - \frac{f_j}{\sqrt{d_i}}\right)^2$$

- The eigenvalue λ and eigenvector $\mathbf{v}$ of $\mathbf{L}_{\mathsf{rw}}$ can be solved from

$$\mathbf{L}\mathbf{v} = \lambda\mathbf{D}\mathbf{v}$$

- The smallest eigenvalue of both $\mathbf{L}_{\mathsf{sym}}$ and $\mathbf{L}_{\mathsf{rw}}$ are 0, with eigen-vectors $\mathbf{1}$ and $\mathbf{D}^{1/2}\mathbf{1}$, respectively.

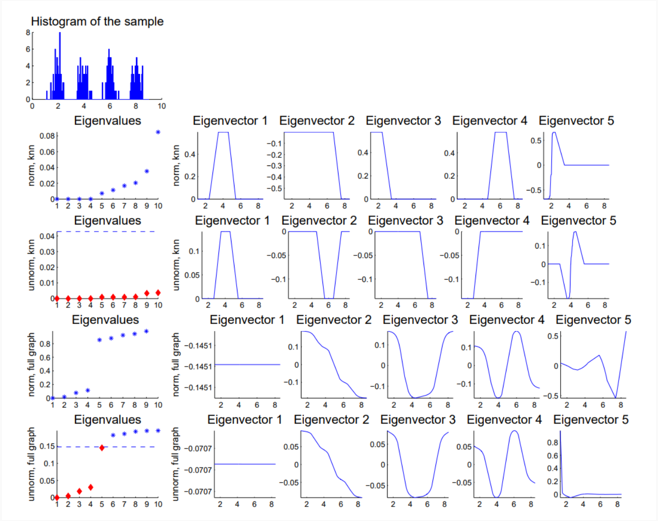
Algorithm

- The spectral clustering is very simple:
  - Construct a weighted adjacency matrix $\mathbf{W}$, using e.g.,

$$w_{ij} = \exp(-\frac{\|x_i - x_j\|^2}{2\sigma^2})$$

  - Compute the Laplacian $\mathbf{L}$ (or normalized versions $\mathbf{L}_{\text{sym}}$, $\mathbf{L}_{\text{rw}}$)
  - Compute the smallest k eigenvectors, denote them collectively as $\mathbf{V}_{n\times k}$
  - Treat $\mathbf{V}_{n\times k}$ as the matrix of the observed data, and perform k-means clustering
  - Output the k cluster labels

Demonstration



Example from Von Luxburg, Ulrike. ”A tutorial on spectral clustering.” Statistics and computing 17, no. 4 (2007): 395-416.

Principal Coordinates Analysis

General Concept

- Principal Coordinates Analysis (PCoA) is also called the classical multidimensional scaling (MDS)
- Given a similarity matrix $\mathbf{S}_{n\times n} = \{s_{ij}\}_{ij}$, we want to construct low-dimensional (k) coordinates $z_1, z_2, \dots, z_n \in \mathbb{R}^k$ such that the inner product of two subjects mimics the corresponding similarity
- More specifically, we minimize the strain function:

$$\text{Strain} = \sum_{ij} \left(s_{ij} - \langle z_i, z_j \rangle\right)^2$$

by solving low-dimensional coordinates $z_1, \dots, z_n$.

Algorithm

- PCoA can also be solved using eigen decomposition:
  - We first obtain the similarity matrix $\mathbf{S}$
  - Let the double centered matrix $\mathbf{B} = -\frac{1}{2}\mathbf{HDH}$, with $\mathbf{H} = \mathbf{I} - \frac{1}{n}\mathbf{1}\mathbf{1}^\mathsf{T}$
  - Perform SVD on $\mathbf{B}$ and obtain the largest k eigenvector $\mathbf{U}_{n\times k}$ and the eigenvalues on the diagonal of $\mathbf{D}_{k\times k}$
  - The principle coordinate matrix is $\mathbf{UD}^{1/2}$
- If the similarity matrix $\mathbf{S}$ is in fact the centered inner product of the original data $\mathbf{X}$, then PCoA is the same as PCA.