Lecture 2: Introduction to Low Rank Approximation, Dimension Reduction, and Clustering

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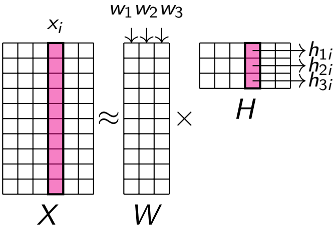
Overview

Linear Algebra is an important foundation in data analytics.

- Constrained low-rank approximations (CLRA) for modeling and algorithm/software development for scalable data analytics



PCA, SVD, LSI, pLSI, K-means
Topic/trend/video tracking
Community structure discovery

Recommendation system, ...

Lecture 2 Outline:

- Introduction to Low Rank Approximation
- Dimension Reduction
- Clustering of data represented in a feature-object matrix (attribute/content): data clustering, topic modeling, ...

Constrained Low Rank Approximations for Scalable Data Analytics

Objectives: Using CLRA,

- Model text and graph analytics problems
- Design, verify, and deploy scalable numerical alg.

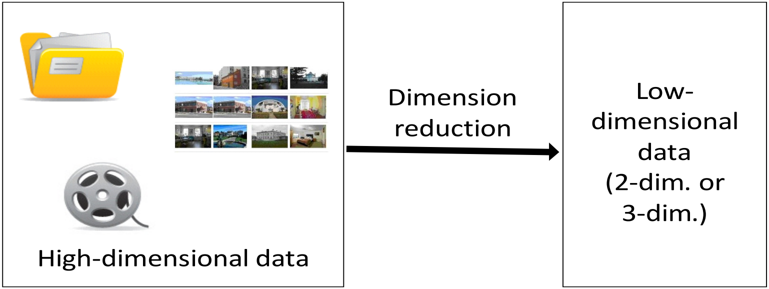
Goal: Orders of magnitude improvements over existing data analytics methods and solutions of higher quality

Why CLRA ?

- Utilize advances in numerical linear algebra and optimization
- Exploit software such as BLAS and LAPACK
- Behavior of algorithms easier to analyze
- Adaptive algorithms for streaming data
- Facilitates design of MPI based algorithms for scalable solutions
- Can easily be modified for various problem demands

Dimension Reduction

- Goal: Represent high-dimensional data in a lower dimension in order to visualize it or to make subsequent computation manageable.
- Input: Data $X = \{x_1, x_2, \ldots, x_n\} \in \mathbb{R}^m$, reduced dimension k
- Output: Reduced-dimensional representation of data $y_1, y_2 \ldots, y_n \in \mathbb{R}^k$
  - Local, Global
  - Linear, Nonlinear
  - Unsupervised, Semi-supervised, Supervised



Curse of dimensionality

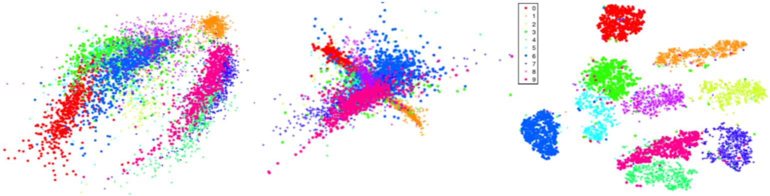
- When dimensionality increases, data bacomes increasingly sparse in the space that it occupies
- Definitions of density and distance between points, which is critical for clustering and outlier detection, become less meaningful

Purpose and Techniques

- Purpose
  - Avoid curse of dimensionality
  - Reduce computational time and memory for algorithms
  - Allow data to be more easily visualized
  - May help to eliminate irrelevant features or reduce noise
- Techniques
  - Feature selection: Finding a subset of the original variables, e.g., features or attributes, which represent the original data.
  - Feature extraction: Transforms the data to a space of fewer dimensions. Different from feature selection, the features does not have to be the features in the original data.
    - Multidimensional scaling (MDS)
    - Principal component analysis (PCA)
    - Latent semantic analysis (LSA)
    - Non-negative matrix factorization (NMF)
    - Linear discriminant analysis (LDA)
    - Isometric Feature Mapping (ISOMAP)
    - Locally Linear Embedding (LLE)
    - Laplacian Eigenmaps
    - T-SNE (T-Distributed Stochastic Neighborhood Embedding) ...

Linear and Nonlinear Methods

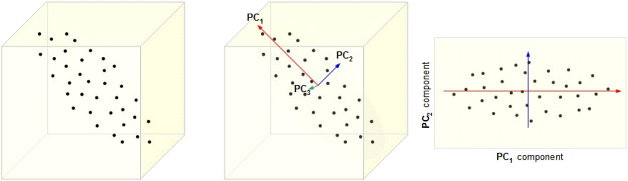
- PCA and SVD are mainly concerned with larger distances
  - Euclidian distance does not reflect similarity in high dim space very well when considering the structure of the data
  - Need methods preserving local structure focusing more on small pairwise distances
- ISOMAP: Geodesic distance in the data space, embedding is a little better
- LLE: Similar to t-SNE, focuses more on small pairwise distances, collapses many points to the center and lets outliers to satisfy the constraints



ISOMAP LLE t-SNE
MNIST vis (Handwritten digits) (van der Maaten and Hilton, JMLR08)

PCA (Principal Component Analysis)

- High level view
  - Seeks the most accurate data representation in a lower dimensional space
  - Preserves as much varience as possible
  - Not suitable for clustered data



Feature Extraction: PCA

- Algorithm
  - Can solve it using SVD
  - Let $X \in \mathbb{R}^{m \times n}$ be the data matrix where $m = \#$ of features, $n = \#$ of data samples.
  - Mean centering: Substract the centroid from every column
  - SVD: $X_c = U \Sigma V^T$ where U and V are orthogonal matrices and Σ is a diagonal matrix containing singular values.
  - Here, the columns of U can be seen as eigenvector of the empirical covarience matrix. ($X_c X_c^T = U \Sigma^2 U^T$)
  - Projection to k-dim. space: $Y = U_k^T X_c = \Sigma_k V_k^T$ (U_k, Σ_k, and V_k are the first k columns of U, Σ, and V respectively)

Feature Extraction: LSA (Latent Semantic Analysis)

- LSA exploits co-occurences of terms in documents to produce a mapping into a latent semantic space
- The new semantic space can find similar documents and relations between terms
- Term-Document Matrix
  - Let's assume we have three documents as following
    - D1: "I like visual analytics"
    - D2: "Visual representations and visual interactions"
    - D3: "Analytical reasoning and visualization"
  - TF+IDF, stop list removal, ...

$$
\begin{array}{c c c}
\text{Terms} & & \begin{array}{ccc} \text{D1} & \text{D2} & \text{D3} \end{array} \\
\begin{array}{c}
\text{analytical} \\ \text{analytics} \\ \text{and} \\ \text{I} \\ \text{interactions} \\ \text{like} \\ \text{reasoning} \\ \text{representations} \\ \text{visual} \\ \text{visualization}
\end{array}
& X = &
\left[\begin{array}{ccc}
0 & 0 & 1 \\
1 & 0 & 0 \\
0 & 1 & 1 \\
1 & 0 & 0 \\
0 & 1 & 0 \\
1 & 0 & 0 \\
0 & 0 & 1 \\
0 & 1 & 0 \\
1 & 2 & 0 \\
0 & 0 & 1
\end{array}\right]
\end{array}
$$

Feature Extraction: LSA (continued)

Algorithm

- Applies SVD on the term-document matrix X
  $X = U_r S_r V_r^T$ where $X \in \mathbb{R}^{m \times n}$, $U_r \in \mathbb{R}^{m \times r}$, $S_r \in \mathbb{R}^{r \times r}$, and $V_r \in \mathbb{R}^{n \times r}$ (r is rank of X)
- Pick the top k largest singular values (in matrix S_r) and its corresponding singular vectors (in matrices U_r and V_r)

Feature Extraction: NMF (Non-negative Matrix Factorization)

Given the a non-negative matrix $X \in \mathbb{R}^{m \times n}$ and an integer $k \ll min\{m, n\}$, find non-negative matrices $W \in \mathbb{R}^{m \times k}$ and $H \in \mathbb{R}^{k \times n}$, which minimizes $\|X - WH\|_F^2 = \sum_i \sum_j (X_{ij} - [WH]_{ij})^2$.

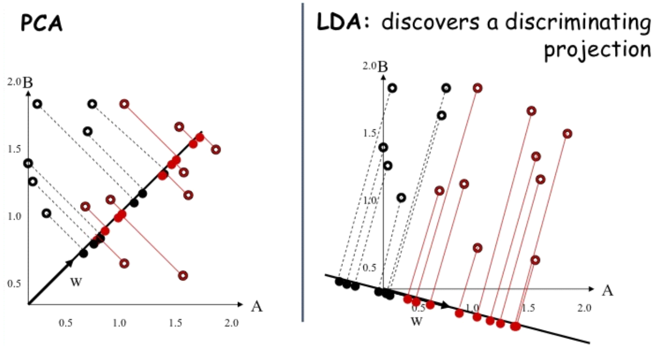
- W: basis for a k-dim space, the ith col of H: k-dim representation of the ith col of X
- Maintaining non-negativity prevents one factor from removing content that another factor contributed. NMF can uncover latent factors with better interpretability.
- Algorithm
  - Nonconvex
  - The factors are not unique
    (e.g., If we have a nonsingular matrix P, where $WP \geq 0$ and $P^{-1}H \geq 0$, then $(\tilde{W} = WP,\ \tilde{H} = P^{-1}H)$ is another solution, e.g. P is a diagonal matrix with positive diagonal elts.

Feature Extraction: LDA(Linear Discriminant Analysis)

P. Howland and HP, TPAMI 2004

- A supervised dimension reduction method for clustered data
- Maximizes between class separation while minimizing data separation within each class
- Algorithm
  - Want a linear transformation $G^T : x \in R^{m\times 1} \to y \in R^{l\times 1}$ assuming X is already clustered into k clusters $X = [X_1, \cdots, X_k]$
  - Two scatter matrices:
    Between-cluster scatter matrix
    $S_b = \sum_{j=1}^{k} \sum_{i\in C_j} (c^{(j)} - c)(c^{(j)} - c)^T$
    Within-cluster scatter matrix
    $S_w = \sum_{j=1}^{k} \sum_{i\in C_j} (x_i - c^{(j)})(x_i - c^{(j)})^T$
    $c^{(j)}$: centroid for the jth cluster, c: global centroid
  - Find G that
    maximizes trace$(G^T S_b G)$ while minimzes trace$(G^T S_w G)$
  - Find G that maximizes trace$((G^T S_w G)^{-1} G^T S_b G)$
  - Solved by a generalized eigenvalue problem

Graphical Example of PCA vs. LDA



(Figure from http://stuff.ttoy.net/cs591o/)

Generalized Singular Value Decomposition (GSVD)

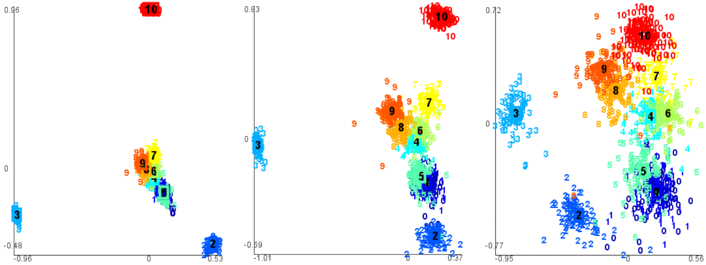
- GSVD: For $K_A \in R^{m \times n}$ with $m \geq n$ and $K_B \in R^{p \times n}$,
  there are $U \in R^{m \times m}$ and $V \in R^{p \times p}$
  with $U^T U = I$ and $V^T V = I$,
  and a nonsingular $X \in R^{n \times n}$ such that
  $U^T K_A X = diag(\alpha_1, \cdots, \alpha_n)$ and $V^T K_B X = diag(\beta, \cdots, \beta_q)$
  where $q = min(p, n)$, $\alpha_i \geq 0$, and $\beta_i \geq 0$.
- Through GSVD, we can solve generalized EVD:
  $\beta_i^2 K_A^T K_A x_i = \alpha_i^2 K_B^T K_B x_i$
- No nonsingularity condition on $K_B^T K_B$ is needed

LDA via GSVD

- $S_t = S_w + S_b$: total scatter matrix = covariance matrix
- PCA solves maximize $trace(G^T S_t G)$
- Letting
  $H_w = [X_1 - c^{(1)} {e^{(1)}}^T, \cdots, X_k - c^{(k)} {e^{(k)}}^T]$ and
  $H_b = [(c^{(1)} - c){e^{(1)}}^T, \cdots, (c^{(k)} - c){e^{(k)}}^T]$,
  we have $S_w = H_w H_w^T$ and $S_b = H_b H_b^T$
- GEVD of $\beta^2 S_b x = \alpha^2 S_w x$ can be solved via GSVD of H_w^T and H_b^T, regardless of nonsingularity of S_w

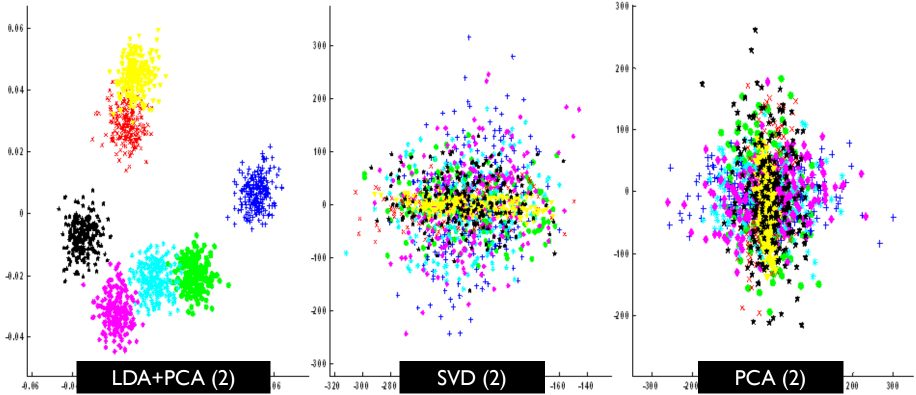
- LDA/GSVD algorithm
- Another way to handle singular S_w: Regularized LDA
  - Used when the data is undersampled, i.e., when # of dim > # of samples.
  - Regularized LDA max $trace((G^T S_w G + \gamma I)^{-1} G^T S_b G)$, where $G^T S_w G + \gamma I$ is guaranteed to be nonsingular for $\gamma > 0$

Application of LDA for 2D vis of clustered data



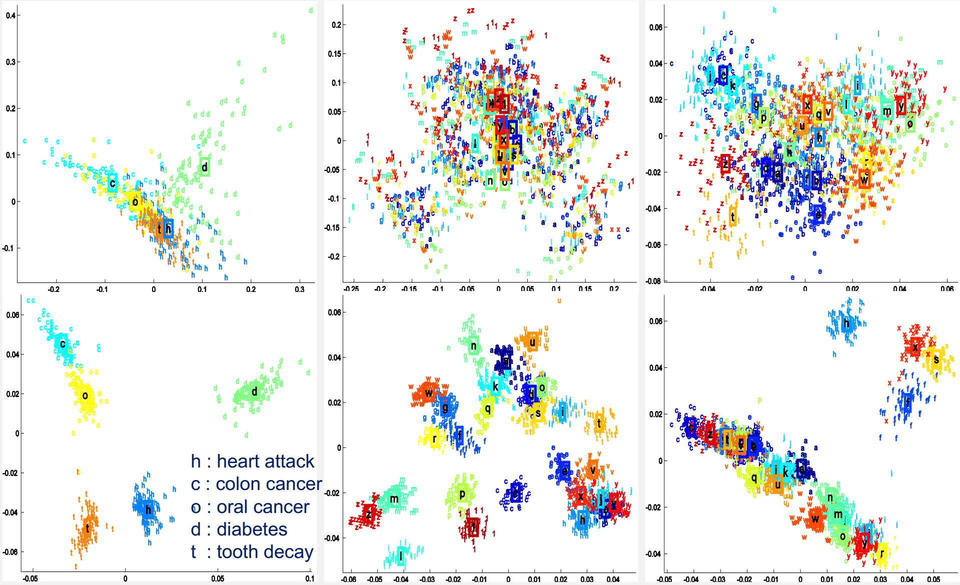
$\gamma = 10^0$ $\gamma = 10^1$ $\gamma = 10^2$

LDA/GSVD FOR 2D REPRESENTATION OF HIGH DIMENSIONAL CLUSTERED DATA



2D representation of 700x1000 data with 7 clusters: LDA vs. SVD vs. PCA
Want to represent data/cluster/outlier info even after a severe dim. reduction

2D VISUALIZATION (PCA VS LDA) OF CLUSTERED TEXT, IMAGE, AUDIO DATA



Medline Data *(Text)* | Facial Data *(Image)* | Spoken Letters *(Audio)*

Clustering

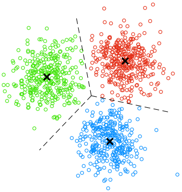
Given an unlabeled data set (no prior knowledge), how can we find grouping structures/patterns hidden in the data?

- Goal: Group *similar* objects together.
- Input: Data $X = [x_1, x_2, \ldots, x_n]$, number of clusters k
- Output: Data partitioning $X_1, X_2, \ldots, X_k$
- It provides an overview of large-scale data, dimension reduced representations, makes subsequent data analytics tasks more efficient.
- Core problem: k basis vectors where each represents a cluster well ? E.g. news articles:

Clustering

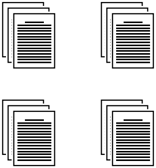
(J. Kim and H. Park, SISC 11; J.Kim, Y. He, and H. Park, JOGO 14, D. Kuang, S. Yun, and H. Park, JOGO 15)

Vector space



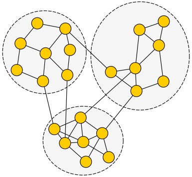
$$\min_{\substack{\mathbf{1}_k^T H = \mathbf{1}_n^T \\ H \in \{0,1\}^{k\times n}}} \|X - WH\|_F$$

Text (Topic Modeling)



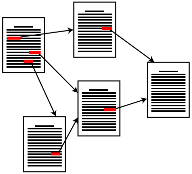
$$\min_{W\geq 0, H\geq 0} \|X - WH\|_F$$

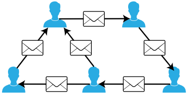
Graph (Community Detection)



$$\min_{H\geq 0} \|S - H^T H\|_F$$

Hybrid





$$\min_{W\geq 0, H\geq 0} \|X - WH\|_F^2 + \alpha \|S - H^T H\|_F^2$$

Clustering

Two most commonly used methods:

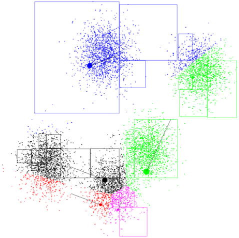
- For feature-data relationship: K-means
- For data-data relatinship: Spectral clustering

Given k initial clustering centroids, K-means iteratively:

- Assigns each data point x_i to the nearest centroid in terms of Euclidean distance (or cosine value for spherical K-means)
- Recomputes k centroids

There are many versions of K-means and other variants such as K-median and K-medoids methods

- Step 0



K-means algorithm for data matrix $X = [x_1, \cdots, x_n]$

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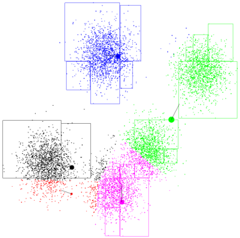

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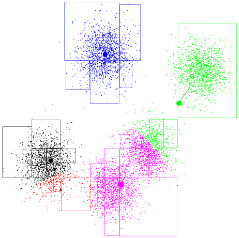
- Step 0
- Step 1
- Step 2



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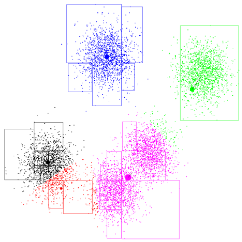
- Step 0
- Step 1
- Step 2
- Step 3



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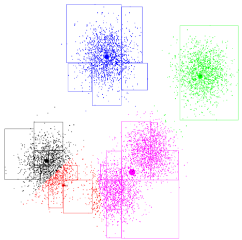
- Step 0
- Step 1
- Step 2
- Step 3
- Step 4



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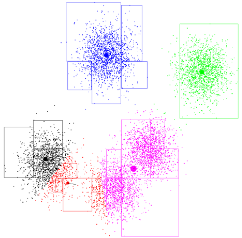
- Step 0
- Step 1
- Step 2
- Step 3
- Step 4
- Step 5



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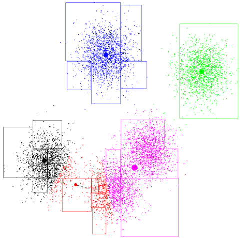
- Step 0
- Step 1
- Step 2
- Step 3
- Step 4
- Step 5
- Step 6



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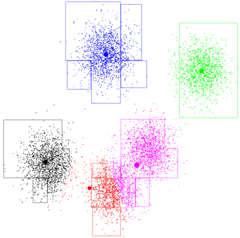
- Step 6
- Step 7



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- Step 0
- Step 1
- Step 2
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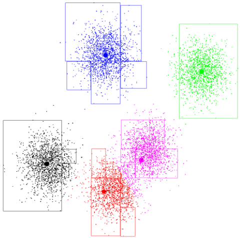
- Step 4
- Step 5
- Step 6
- Step 7
- Step 8



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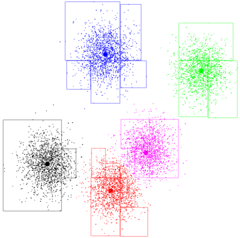


Given a notion of similarity $s_{ij} \geq 0$ between all pairs of data points, we form a similarity graph $G = (V, E)$.

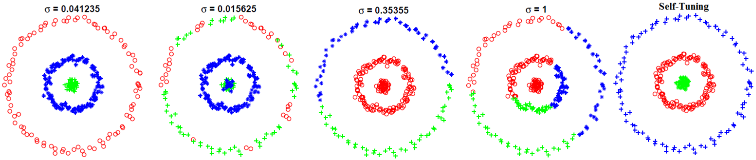
- Similarity Graph
  - The ε-neighborhood graph
    - Connect points whose pairwise distance are smaller than ε.
  - k-nearest neighbor graph (KNN graph)
    - Connect node x_i and x_j if x_j is among the k_n-nearest neighbors of x_i.
  - Mutual k-nearest neighbor graph (mutual KNN graph)
    - Connect node x_i and x_j if x_j is among the k_n-nearest neighbors of x_i and x_i is among the k-nearest neighbors of x_j.
  - Fully connected graph
    - Connect all points with an edge and assign the weight as pairwise positive similarity value.

[Von Luxburg, 2007]

A *self-tuned* way to define edge weight: [Zelnik-Manor and Penora, NIPS, 2004]

- $$s_{ij} = \exp\left(-\frac{\|x_i - x_j\|_2^2}{2\sigma_i \sigma_j}\right)$$

  where the *local scale* σ_i is the distance between x_i and its $\hat{k}$-th neighbor.



Spectral Clustering

Which similarity graph to choose? How to choose parameters in the similarity graph?

- A safe way is to build a *connected* graph.
- Choose ϵ, k_n, etc. so that the graph is connected.
- KNN graph is often a good starting point.
- The edge weight can be defined as the RBF kernel:

$$s_{ij} = \exp\left(-\frac{\|x_i - x_j\|_2^2}{2\sigma^2}\right)$$

- But how to choose σ?
- Note: There is no theoretically principled way to choose the type of graph and parameters. And the clustering result is very sensitive to k and σ.

[Von Luxburg, 2007]

Which eigenvalues to compute?

Ratio cut: $\min \sum_{p=1}^{k} \frac{\sum_{i\in V_p, j\in V-V_p} W_{ij}}{\lvert V_p\rvert}$
k smallest eigenvalues of L

Ratio association: $\max \sum_{p=1}^{k} \frac{\sum_{i\in V_p, j\in V_p} W_{ij}}{\lvert V_p\rvert}$
k largest eigenvalues of W

Normalized cut: $\min \sum_{p=1}^{k} \frac{\sum_{i\in V_p, j\in V-V_p} W_{ij}}{\sum_{i\in V_p, j\in V} W_{ij}}$ $\Leftrightarrow \max \sum_{p=1}^{k} \frac{\sum_{i\in V_p, j\in V_p} W_{ij}}{\sum_{i\in V_p, j\in V} W_{ij}}$
k smallest eigenvalues of $D^{-1/2}LD^{-1/2}$ $\Leftrightarrow$ k largest eigenvalues of $D^{-1/2}WD^{-1/2}$

Spectral Clustering

The main tool for spectral clustering is the affinity matrix S and the graph Laplacian matrix L (n: number of nodes in graph)

- $S \in \mathbb{R}^{n \times n}$ contains edge weights between all connected pairs
- $D \in \mathbb{R}^{n \times n}$ is a diagonal matrix with degrees $d_1, d_2, \ldots, d_n$ on the diagonal: $d_i = \sum_{j=1}^{n} s_{ij}$
- L is the graph Laplacian matrix: $L = D - S$
  - Symmetric Positive Semi-definite
  - For every vector $f \in \mathbb{R}^n$, $f^T L f = \frac{1}{2} \sum_{i,j=1}^{n} s_{ij}(f_i - f_j)^2$
  - The smallest eigenvalue is 0 and its eigenvector has all ones $\vec{1}$
  - All eigenvalues are real and nonnegative $0 = \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$
  - The multiplicity of the eigenvalue 0 is equal to the number of connected components in graph. Ex. $L = \begin{pmatrix} L_1 & 0 & 0 \\ 0 & L_2 & 0 \\ 0 & 0 & L_3 \end{pmatrix}$

Spectral Clustering

(One possible) Algorithm:

1. Input: Data points $x_1, \cdots, x_n$, number of clusters k
2. Construct a similarity graph and compute matrices S and L.
3. Compute the smallest k eigenvectors $u_1, u_2, \ldots, u_k$ of L.
4. Let $U = \begin{bmatrix} u_1 & u_2 & \ldots & u_k \end{bmatrix} \in \mathbb{R}^{n \times k}$.
5. For $i = 1, 2, \ldots, n$, let $y_i \in \mathbb{R}^k$ be the vector corresponding to the i-th row of U.
6. Cluster the points $(y_i)_{i=1,2,\ldots,n}$ with the k-means algorithms to clusters $C_1, C_2, \ldots, C_k$.
7. Output: Partitioned data $X_j = \{i : y_i \in C_j\}$.

From objective functions to eigenvalues: Spectral relaxation

- Normalized cut objective: $\min \sum_{p=1}^{k} \frac{\sum_{i\in V_p, j\in V-V_p} S_{ij}}{\sum_{i\in V_p, j\in V} S_{ij}}$
- Define cluster indicator vector:
  $h_p = D^{1/2}[0,\cdots,0,1,\cdots,1,0,\cdots,0]^T$ with n_p 1's
- Define normalized indicator $y_p = h_p/\|h_p\|_2$, and rewrite J:

$$J = \sum_{p=1}^{k} y_p^T L y_p = \mathrm{trace}(Y^T D^{-1/2} L D^{-1/2} Y)$$

  where $Y = [y_1, \cdots, y_k]$
- Relax the constraints of Y to be $Y^T Y = I$:

$$\min_{Y^T Y = I} \mathrm{trace}(Y^T D^{-1/2} L D^{-1/2} Y)$$

- By *Ky Fan* theorem, the optimal Y is the eigenvectors corresponding to the smallest eigenvalues of $D^{-1/2} L D^{-1/2}$