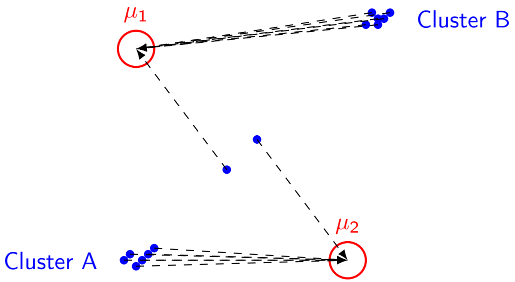
IEMS 304 Lecture 8: Unsupervised Learning

Yiping Lu
yiping.lu@northwestern.edu

Industrial Engineering & Management Sciences
Northwestern University

k-means

Iteration 1: Initialization & Forced Assignment



Assignment Summary (Iteration 1):

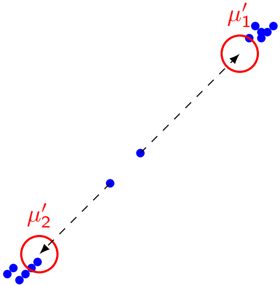
- $\mu_1 = (1, 4.5)$ gets: all Cluster B points (6 pts) + ambiguous point $(2.5, 2.5)$ [total 7 pts].
- $\mu_2 = (4.5, 1)$ gets: all Cluster A points (6 pts) + ambiguous point $(3, 3)$ [total 7 pts].

Updated centroids (computed as the mean):

$$\mu_1' = \left(\frac{30+2.5}{7}, \frac{30+2.5}{7}\right) \approx (4.643,\ 4.643)$$

$$\mu_2' = \left(\frac{6.3+3}{7}, \frac{6.3+3}{7}\right) \approx (1.329,\ 1.329)$$

Iteration 2: Reassignment



Reassignment (Iteration 2):

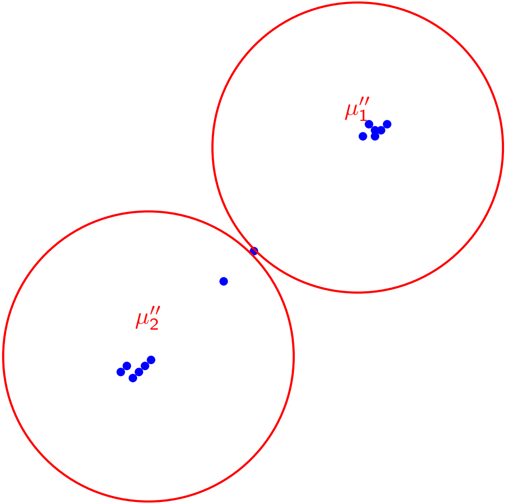
- $(2.5, 2.5)$ switches from μ_1 to μ_2' (closer to $(1.329, 1.329)$).
- $(3, 3)$ switches from μ_2 to μ_1' (closer to $(4.643, 4.643)$).

New centroids:

$$\mu_1'' = \left(\frac{30+3}{7},\ \frac{30+3}{7}\right) = \left(\frac{33}{7},\ \frac{33}{7}\right) \approx (4.714,\ 4.714)$$

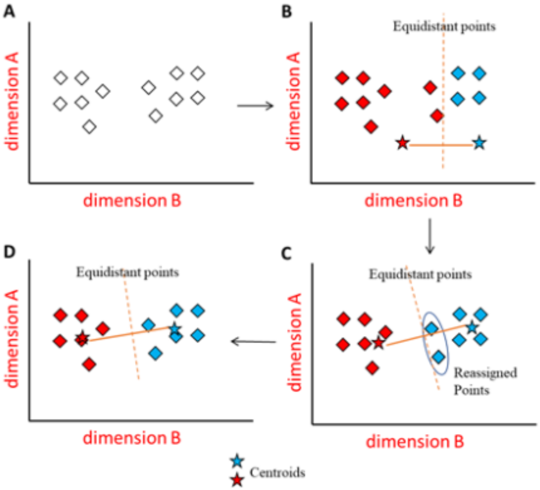
$$\mu_2'' = \left(\frac{6.3+2.5}{7},\ \frac{6.3+2.5}{7}\right) = \left(\frac{8.8}{7},\ \frac{8.8}{7}\right) \approx (1.257,\ 1.257)$$

Iteration 3: Convergence



Convergence: With centroids $\mu_1'' \approx (4.714, 4.714)$ and $\mu_2'' \approx (1.257, 1.257)$, all data points are now correctly grouped according to their true clusters.

$k-$means



A
dimension A
dimension B
B
Equidistant points
dimension A
dimension B
D
Equidistant points
dimension A
dimension B
C
Equidistant points
dimension A
Reassigned
Points
dimension B
Centroids

$k-$means as Optimization

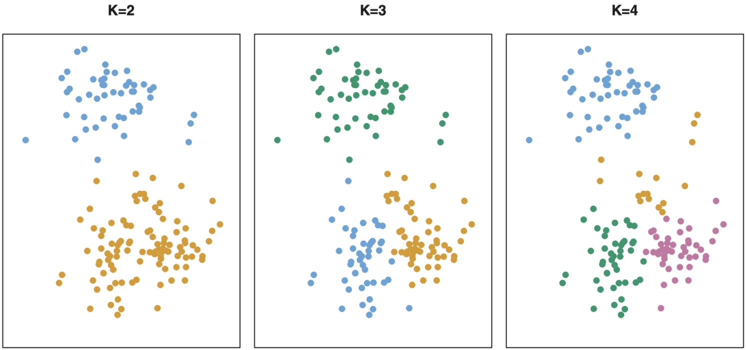
$k-$means aims to minimize the total within cluster (square) distance

$$\min_{\{C_j\},\{\mu_j\}} \sum_{j=1}^{k} \sum_{x \in C_j} \|x - \mu_j\|^2$$

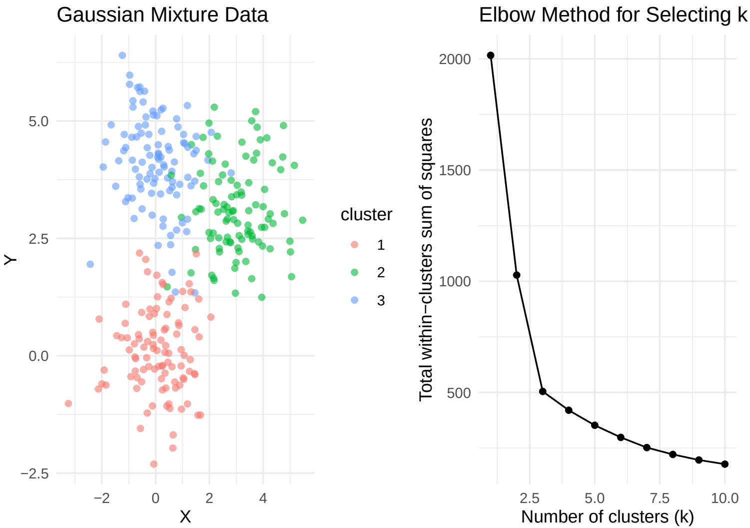
$k-$means as alternating direction optimization algorithm

- **Assignment:** Assign each x to its nearest μ_j (minimizes distance).
- **Update:** Recompute μ_j as the mean of C_j (minimizes variance).

Wrong k can be Problematic

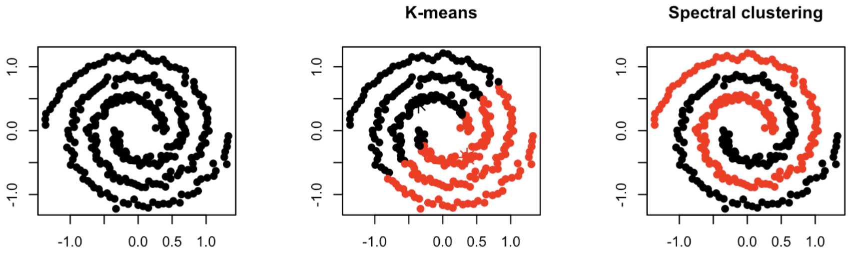


How to Select k: Elbow Effect



Spectral Clustering

Spectral Clustering



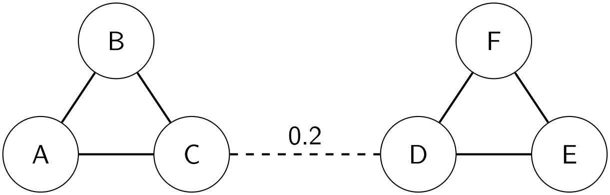
Spectral Clustering

We first represent data as a weighted graph $G(V, E)$ with weights w_{ij}.

Consider the Dirichlet form,

$$\frac{1}{2}\sum_{i,j} w_{ij}\big(f(i) - f(j)\big)^2 = f^T L f, \quad \text{(Why?)}$$

where L is the graph Laplacian defined as $L = D - W$ (where D is the degree matrix).



What would happen if we minimizing this form?

Quadratic Function as a Quadratic Form

$$v^T A v = \begin{pmatrix} x & y \end{pmatrix} \begin{pmatrix} 3 & 2 \\ 2 & 2 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = 3x^2 + 2xy + 2xy + 2y^2 = 3x^2 + 4xy + 2y^2.$$

Why is the Dirichlet Form Equal to $f^T L f$?

Consider the Dirichlet form:

$$\frac{1}{2}\sum_{i,j} w_{ij}\big(f(i)-f(j)\big)^2 = \frac{1}{2}\sum_{i,j} w_{ij}\Big[f(i)^2 - 2f(i)f(j) + f(j)^2\Big].$$

- terms involving $f(i)^2$:

$$\frac{1}{2}\Big(\sum_{i,j} w_{ij}f(i)^2 + \sum_{i,j} w_{ij}f(j)^2\Big)$$

$$= \sum_i f(i)^2 \sum_j w_{ij} = \sum_i d_i f(i)^2.$$

- The cross term simplifies to:

$$-\sum_{i,j} w_{ij}f(i)f(j).$$

$$\frac{1}{2}\sum_{i,j} w_{ij}\big(f(i)-f(j)\big)^2 = \sum_i d_i f(i)^2 - \sum_{i,j} w_{ij}f(i)f(j).$$

At the same time,

$$f^T L f = \sum_i d_i f(i)^2 - \sum_{i,j} w_{ij}f(i)f(j), \text{ where } L = D - W,$$

Understanding the Dirichlet Form

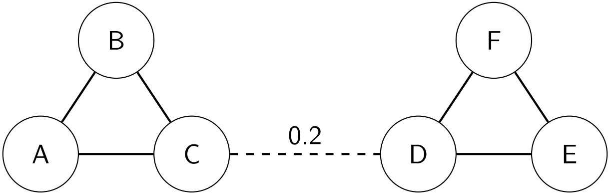
Definition

The Dirichlet form on a graph is defined as:

$$\frac{1}{2}\sum_{i,j} w_{ij}(f(i) - f(j))^2 = f^T L f.$$

- It sums the squared differences of the function values $f(i)$ over every edge, weighted by w_{ij}.
- A small value of $f^T L f$ indicates that neighboring nodes (with high similarity w_{ij}) have similar function values.
- Minimizing the Dirichlet form under constraints leads to smooth functions on the graph, thus revealing inherent cluster structure.

Computing the Graph Laplacian



Step 1: Define the Matrices

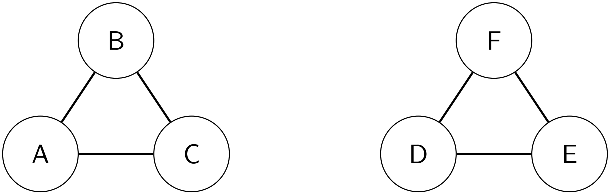
- **Weighted Adjacency Matrix W:** For each edge (i, j), $w(i, j) = 1$ except for the edge between C and D where $w(C, D) = 0.2$.
- **Degree Matrix D:** Diagonal with $d_A = 2, d_B = 2, d_C = 2.2, d_D = 2.2, d_E = 2, d_F = 2$

Step 2: Compute the Graph Laplacian

$$L = D - W$$

$$= \begin{pmatrix} 2 & -1 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ -1 & -1 & 2.2 & -0.2 & 0 & 0 \\ 0 & 0 & -0.2 & 2.2 & -1 & -1 \\ 0 & 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & -1 & 2 \end{pmatrix}.$$

Computing the Graph Laplacian



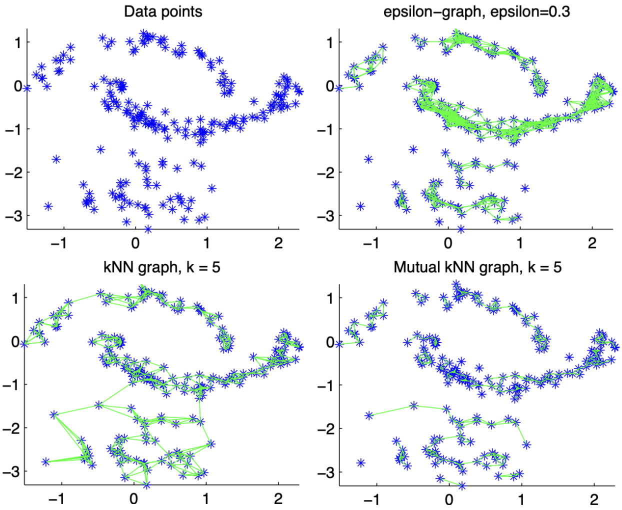
What is the smallest eigenvalue/eigenvectors of the graph laplacian?
What would happen if we have l-connected component

Spectral Clustering

$$\max f^\top L f \qquad \text{s.t. } f^\top \mathbb{1} = 0, \|f\|_2 = 1$$

Then run a $k-$means on the spectral clustering representation f. (homework)

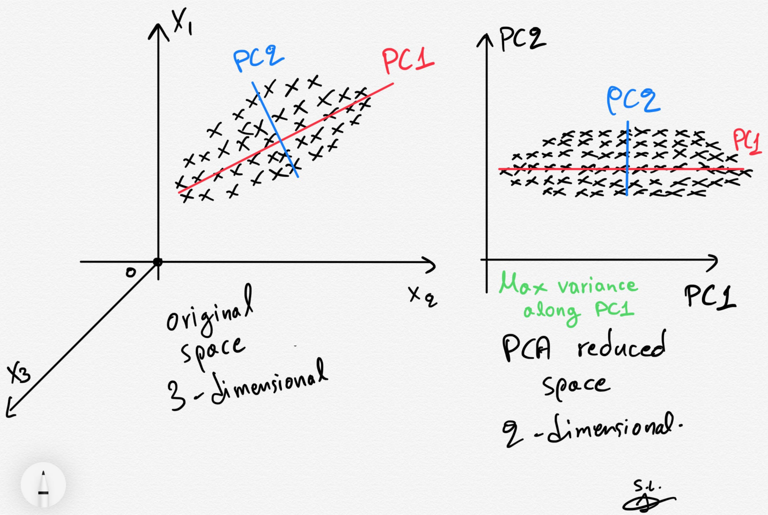
Graph



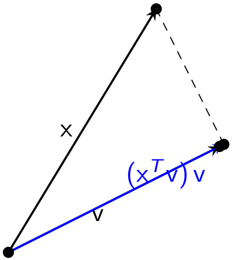
Data points
epsilon−graph, epsilon=0.3
kNN graph, k = 5
Mutual kNN graph, k = 5
1
0
−1
−2
−3
−1
0
1
2

Dimension Reduction

Principal Component Analysis (PCA)



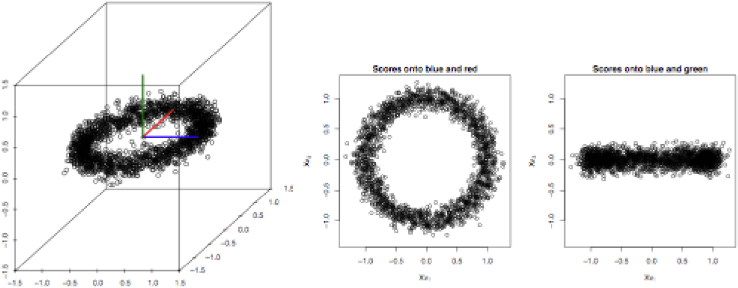
Projection



- $x^T v \in \mathbb{R}$: score
- $(x^T v)\,v \in \mathbb{R}^p$: projection

Not All Projection are the Same

Example: $X \in \mathbb{R}^{2000 \times 3}$, and $v_1, v_2, v_3 \in \mathbb{R}^3$ are the unit vectors parallel to the coordinate axes



Not all linear projections are equal! What makes a good one?

PCA: Preserve Most Information

We have n d-dimensional data points $x_1, x_2, \ldots, x_n \in \mathbb{R}^d$ and a parameter $k \in \{1, 2, \ldots, d\}$. We assume that the data is centered, meaning that $\sum_{i=1}^{n} x_i = 0$. (How to do that?)

AIM. Find directions that maximize the information preserved
The output of the method is defined as k orthonormal vectors $v_1, v_2, \ldots, v_k$ — the "top k principal components" — that maximize the objective function :

$$\frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{k} (x_i \cdot v_j)^2 .$$

Question: Why we want the principal components orthonormal?

Review: Projection Under Orthonormal Basis

Let $A = [v_1, \cdots, v_k]$ where $v_1, \cdots, v_k$ are orthonormal. **Remind.** Least square solution: $A\beta \approx b$, then $\beta = (A^\top A)^{-1} A^\top b$ Then $A\beta = A(A^\top A)^{-1} A^\top b$

Review. Orthonormal means $A^\top A = I$

Check. Project b to $\text{span}\{v_1, \cdots, v_k\}$ means

$$\langle v_1, b\rangle v_1 + \langle v_2, b\rangle v_2 + \cdots + \langle v_k, b\rangle v_k$$

Matrix Formulation

Matrix Formulation: Define $V \in \mathbb{R}^{d \times k}$ with columns $\mathrm{v}_1, \ldots, \mathrm{v}_k$, representing the k principal components.

The total variance captured when projecting the data onto the subspace spanned by V is

$$\frac{1}{n}\|XV\|_F^2 = \mathrm{tr}\left(V^T\left(\frac{1}{n}X^TX\right)V\right) = \mathrm{tr}(V^TSV),$$

where $S = \frac{1}{n}X^TX$ is the covariance matrix.

Note that $\|A\|_F^2 = \mathrm{tr}(A^TA)$ For $A = XV$, we have:

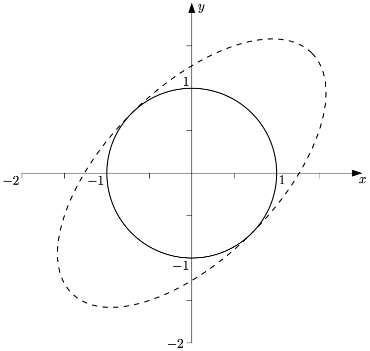
$$\|XV\|_F^2 = \mathrm{tr}((XV)^T(XV)) = \mathrm{tr}(V^TX^\top XV). \qquad (\text{for } \mathrm{tr}(AB) = \mathrm{tr}(BA))$$

$$\max_{V \in \mathbb{R}^{d \times k}} \mathrm{tr}(V^TSV) \quad \text{subject to} \quad V^TV = I_k.$$

Matrix Formulation

Covariance Matrix: Rotation on Principal Component

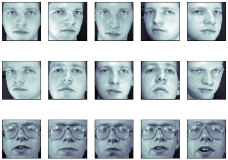
$$\begin{pmatrix} \frac{3}{2} & -\frac{1}{2} \\ \frac{1}{2} & \frac{3}{2} \end{pmatrix} = \underbrace{\begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}}_{\text{rotate back } 45^\circ} \cdot \underbrace{\begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix}}_{\text{stretch}} \cdot \underbrace{\begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}}_{\text{rotate clockwise } 45^\circ}$$

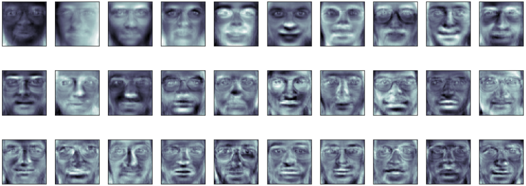


PCA as Top Eigenvectors

PCA boils down to computing the k eigenvectors of the covariance matrix $X^\top X$ that have the largest eigenvalues.

Eigen-Face





The components ("eigenfaces") are ordered by their importance from top-left to bottom-right. We see that the first few components seem to primarily take care of lighting conditions; the remaining components pull out certain identifying features: the nose, eyes, eyebrows, etc.