CSCI 4360/6360 Data Science II

Spectral Clustering

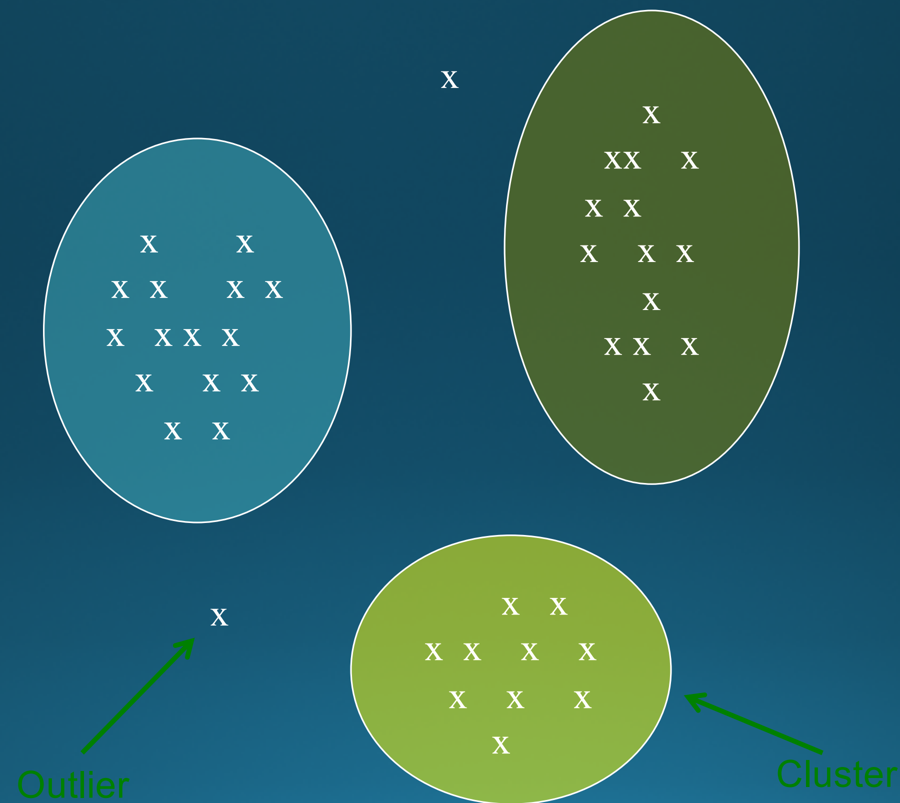
High Dimensional Data

- **Given a cloud of data points we want to understand its structure**

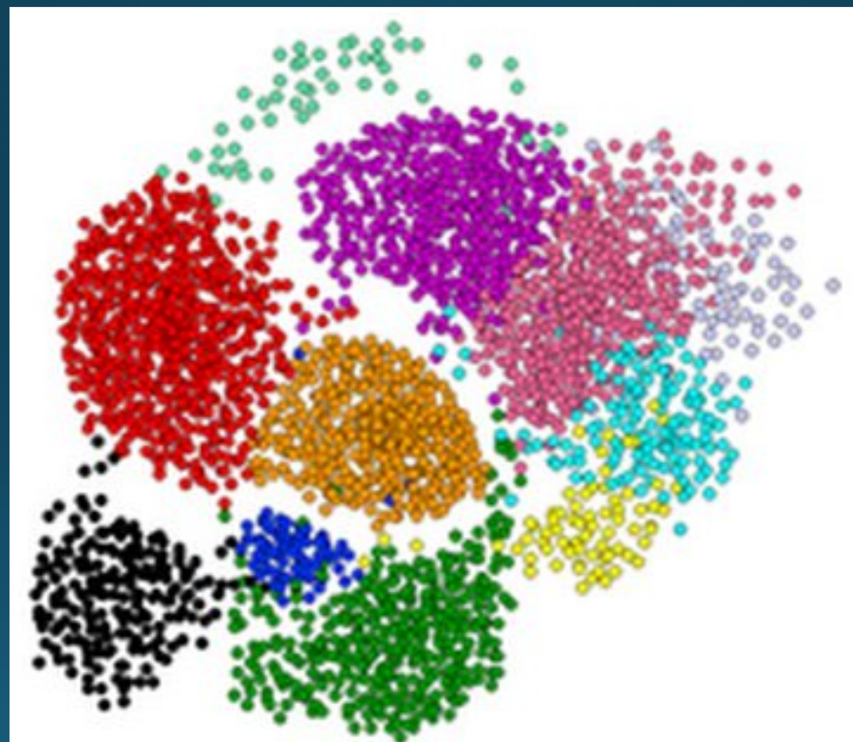
The Problem of Clustering

- Given a **set of points**, with a notion of **distance** between points, **group the points** into some number of ***clusters***, so that
  - Members of a cluster are close/similar to each other
  - Members of different clusters are dissimilar
- **Usually:**
  - Points are in a high-dimensional space
  - Similarity is defined using a distance measure
    - Euclidean, Cosine, Jaccard, edit distance, …

Example: Clusters & Outliers



Clustering is a hard problem!



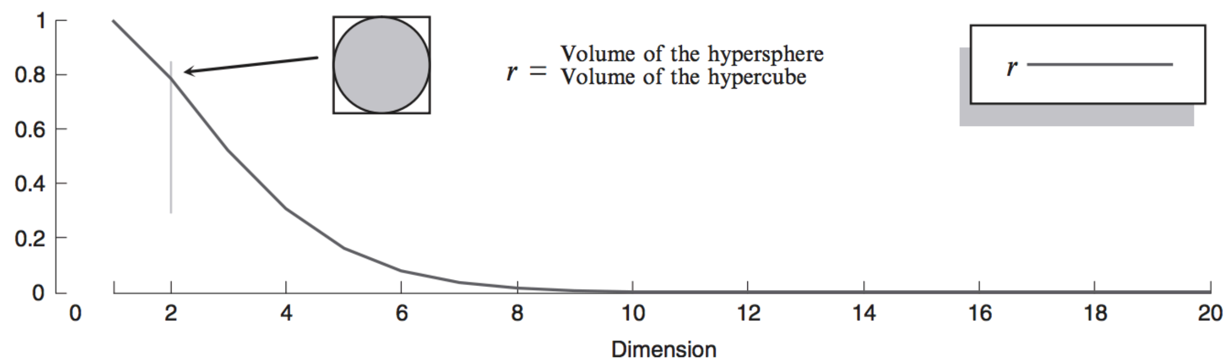
Why is it hard?

- Clustering in two dimensions looks easy
- Clustering small amounts of data looks easy
- And in most cases, looks are not deceiving

- Many applications involve not 2, but 10 or 10,000 dimensions
- **High-dimensional spaces look different:** Almost all pairs of points are at about the same distance

Curse of dimensionality

- "Vastness" of Euclidean space



Curse of Dimensionality. Figure 1. The ratio of the volume of the hypersphere enclosed by the unit hypercube. The most intuitive example, the unit square and unit circle, are shown as an inset. Note that the volume of the hypersphere quickly becomes irrelevant for higher dimensionality

http://link.springer.com/referenceworkentry/10.1007%2F978-0-387-30164-8_192

Clustering Problem: Galaxies

- A catalog of 2 billion "sky objects" represents objects by their radiation in 7 dimensions (frequency bands)
- Problem: Cluster into similar objects, e.g., galaxies, nearby stars, quasars, etc.
- Sloan Digital Sky Survey

Clustering Problem: Music CDs

- **Intuitively: Music divides into categories, and customers prefer a few categories**
  - But what are categories really?

- Represent a CD by a set of customers who bought it:

- Similar CDs have similar sets of customers, and vice-versa

Clustering Problem: Music CDs

Space of all CDs:

- Think of a space with one dimension for each customer
  - Values in a dimension may be 0 or 1 only
  - A CD is a point in this space $(x_1, x_2, \ldots, x_k)$, where $x_i = 1$ iff the i^{th} customer bought the CD
- For Amazon, the dimension is tens of millions
- **Task:** Find clusters of similar CDs

Clustering Problem: Documents

Finding topics:

- Represent a document by a vector $(x_1, x_2, \ldots, x_k)$, where $x_i = 1$ iff the i th word (in some order) appears in the document
  - It actually doesn't matter if k is infinite; i.e., we don't limit the set of words

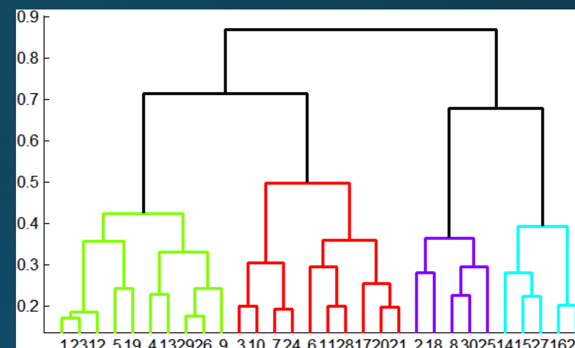
- **Documents with similar sets of words may be about the same topic**

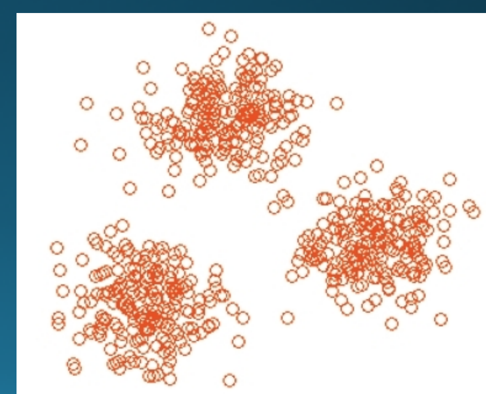
Cosine, Jaccard, and Euclidean

- **As with CDs we have a choice when we think of documents as sets of words or shingles:**
  - **Sets as vectors:** Measure similarity by the **cosine distance**
  - **Sets as sets:** Measure similarity by the **Jaccard distance**
  - **Sets as points:** Measure similarity by **Euclidean distance**

Overview: Methods of Clustering

- **Hierarchical:**
  - **Agglomerative** (bottom up):
    - Initially, each point is a cluster
    - Repeatedly combine the two "nearest" clusters into one
  - **Divisive** (top down):
    - Start with one cluster and recursively split it

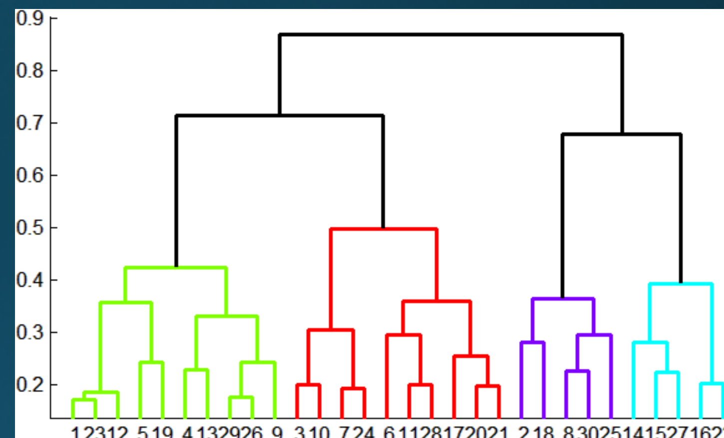




- **Point assignment:**
  - Maintain a set of clusters
  - Points belong to "nearest" cluster

Hierarchical Clustering

- **Key operation:**
  Repeatedly combine two nearest clusters

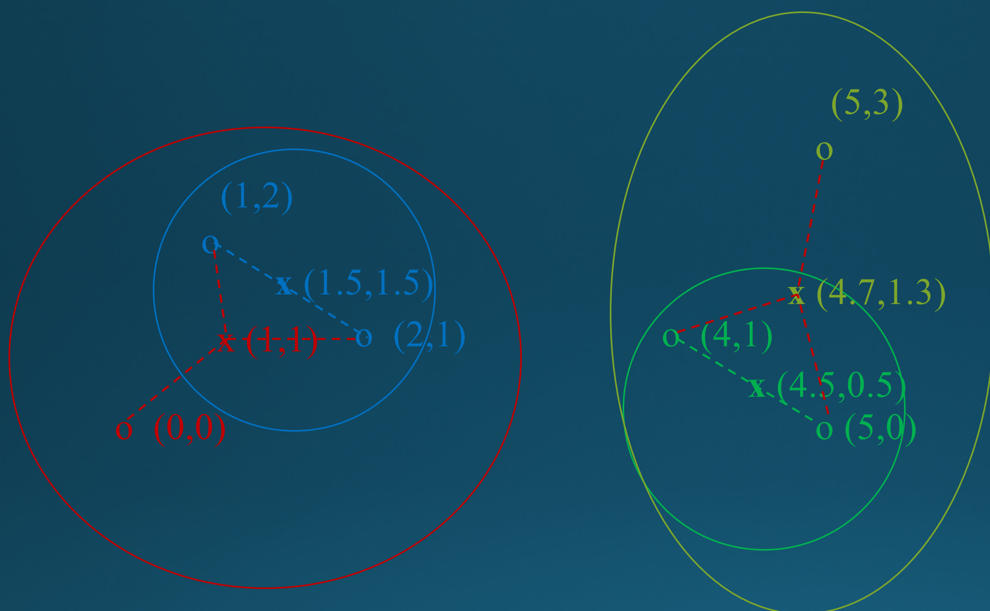


- **Three important questions:**
  - **1)** How do you represent a cluster of more than one point?
  - **2)** How do you determine the “nearness” of clusters?
  - **3)** When to stop combining clusters?

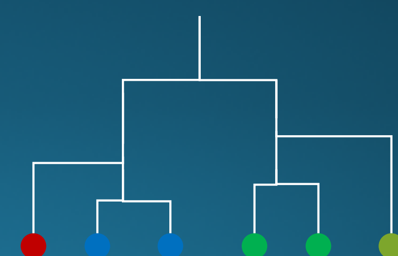
Hierarchical Clustering

- **Key operation: Repeatedly combine two nearest clusters**
- **(1) How to represent a cluster of many points?**
  - Key problem: As you merge clusters, how do you represent the "location" of each cluster, to tell which pair of clusters is closest?
- Euclidean case: each cluster has a *centroid* = average of its (data)points
- **(2) How to determine "nearness" of clusters?**
  - Measure cluster distances by distances of centroids

Example: Hierarchical clustering



Data:
o … data point
x … centroid



Dendrogram

And in the Non-Euclidean Case?

What about the Non-Euclidean case?

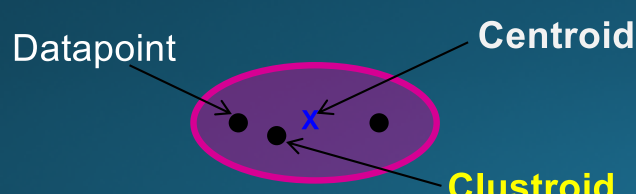
- The only "locations" we can talk about are the points themselves
  - i.e., there is no "average" of two points

- **Approach 1:**
  - **(1) How to represent a cluster of many points?**
    clustroid = (data)point "***closest***" to other points
  - **(2) How do you determine the "nearness" of clusters?** Treat clustroid as if it were centroid, when computing inter-cluster distances

"Closest" Point?

- **(1) How to represent a cluster of many points?**
  clustroid = point "***closest***" to other points
- **Possible meanings of "closest":**
  - Smallest maximum distance to other points
  - Smallest average distance to other points
  - Smallest sum of squares of distances to other points
    - For distance metric ***d*** clustroid ***c*** of cluster ***C*** is:

$$\min_{c} \sum_{x \in C} d(x,c)^2$$



Cluster on
3 datapoints

Centroid is the avg. of all (data)points in the cluster. This means centroid is an "artificial" point.
Clustroid is an **existing** (data)point that is "closest" to all other points in the cluster.

Defining "Nearness" of Clusters

- **(2) How do you determine the "nearness" of clusters?**
  - **Approach 2:**
    Intercluster distance = minimum of the distances between any two points, one from each cluster
  - **Approach 3:**
    Pick a notion of "**cohesion**" of clusters, *e.g.*, maximum distance from the clustroid
    - Merge clusters whose *union* is most cohesive

Cohesion

- **Approach 3.1:** Use the **diameter** of the merged cluster = maximum distance between points in the cluster
- **Approach 3.2:** Use the **average distance** between points in the cluster
- **Approach 3.3:** Use a **density-based approach**
  - Take the diameter or avg. distance, e.g., and divide by the number of points in the cluster

Implementation

- **Naïve implementation of hierarchical clustering:**
  - At each step, compute pairwise distances between all pairs of clusters, then merge
  - $O(N^3)$

- Careful implementation using priority queue can reduce time to $O(N^2 \log N)$
  - **Still too expensive for really big datasets that do not fit in memory**

k–means Algorithm(s)

- Assumes Euclidean space/distance
- Start by picking ***k***, the number of clusters
- Initialize clusters by picking one point per cluster
  - **Example:** Pick one point at random, then ***k*-1** other points, each as far away as possible from the previous points

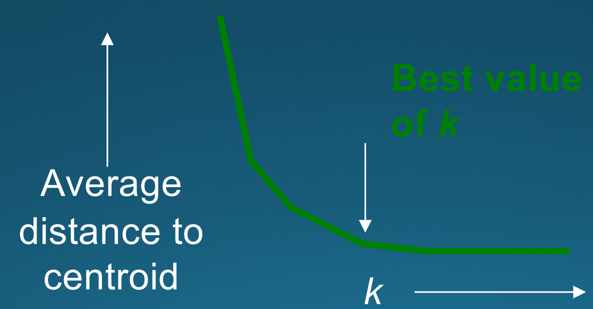
Populating Clusters

- **1)** For each point, place it in the cluster whose current centroid it is nearest
- **2)** After all points are assigned, update the locations of centroids of the ***k*** clusters
- **3)** Reassign all points to their closest centroid
  - Sometimes moves points between clusters
- **Repeat 2 and 3 until convergence**
  - **Convergence:** Points don't move between clusters and centroids stabilize

Getting the *k* right

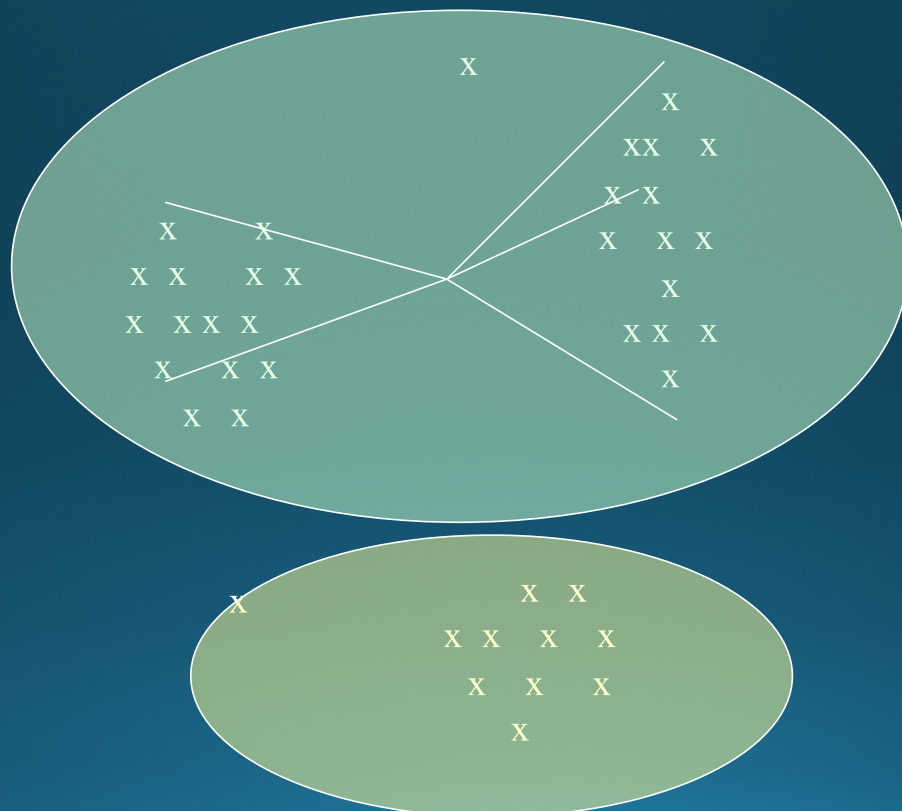
How to select *k*?

- Try different **k**, looking at the change in the average distance to centroid as **k** increases
- Average falls rapidly until right **k**, then changes little



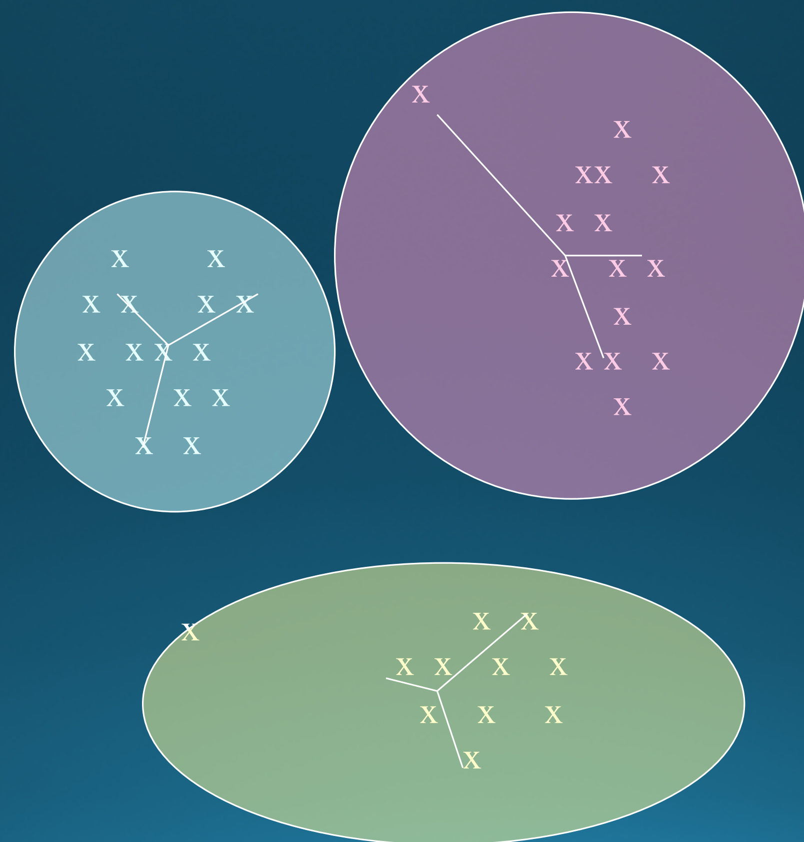
Example: Picking *k*

Too few;
many long distances to centroid.



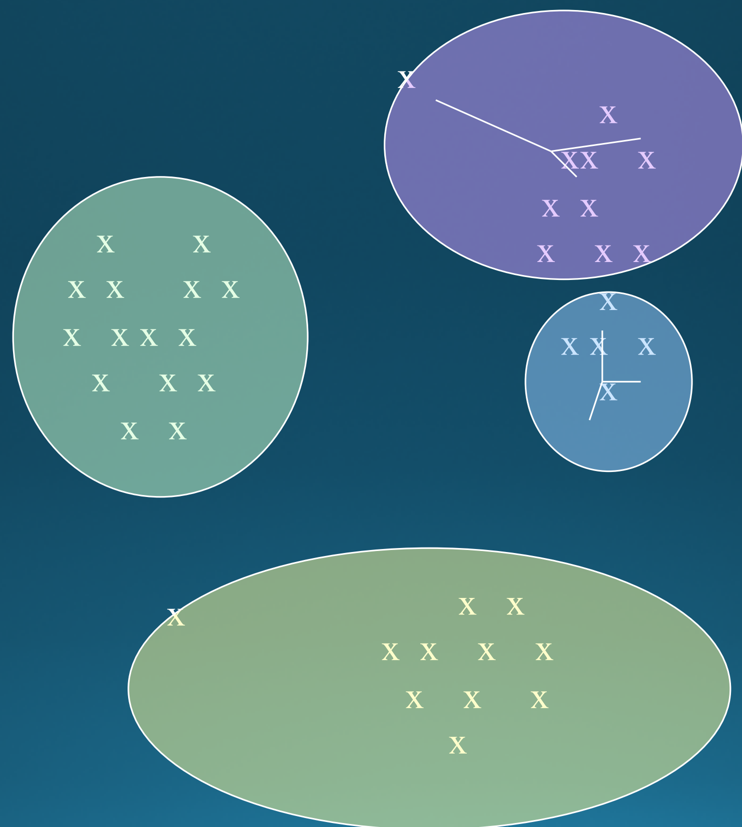
Example: Picking *k*

Just right;
distances
rather short.



Example: Picking *k*

Too many;
little improvement
in average
distance.

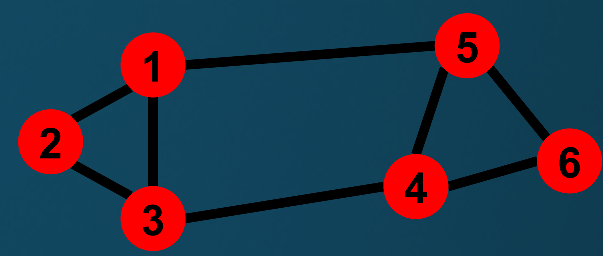


More K-means examples

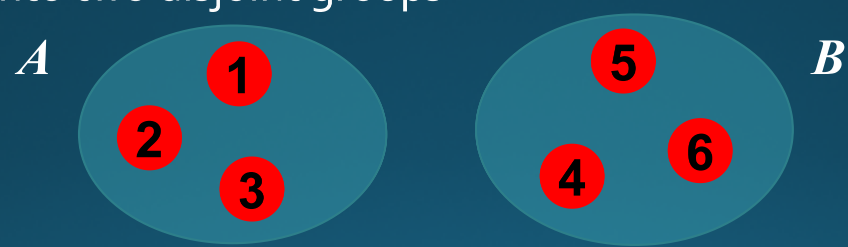
- http://www.naftaliharris.com/blog/visualizing-k-means-clustering/

Graph Partitioning

- **Undirected graph**



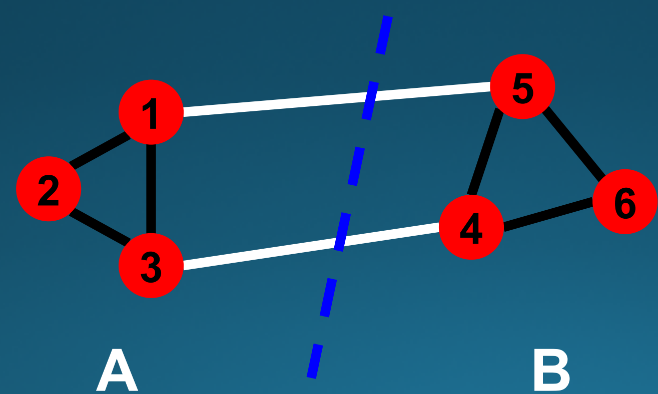
- **Bi-partitioning task:**
  - Divide vertices into two disjoint groups



- **Questions:**
  - How can we define a "good" partition of ?
  - How can we efficiently identify such a partition?

Graph Partitioning

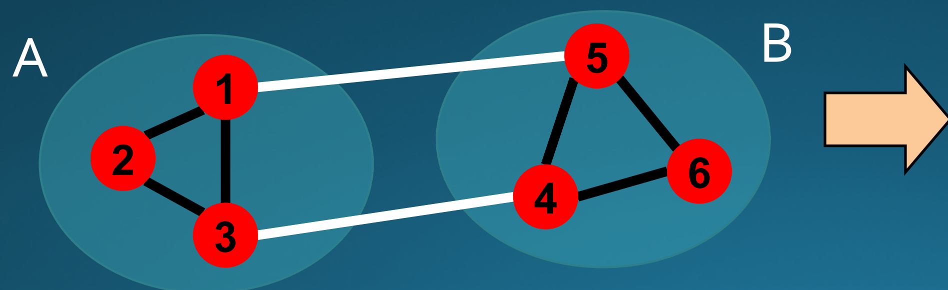
- **What makes a good partition?**
  - Maximize the number of within-group connections
  - Minimize the number of between-group connections



Graph Cuts

- **Express partitioning objectives as a function of the "edge cut" of the partition**
- **Cut:** Set of edges with only one vertex in a group:

$$cut(A,B) = \sum_{i \in A, j \in B} w_{ij}$$



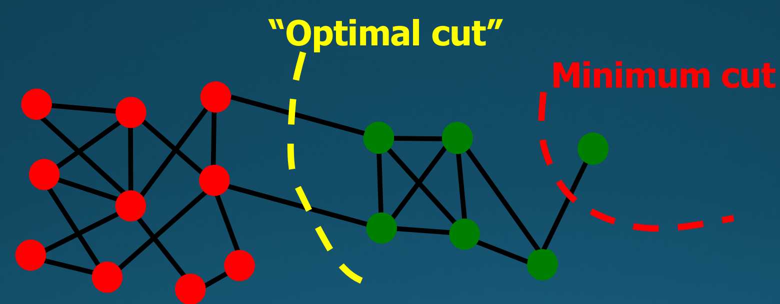
$cut(A,B) = 2$

Graph Cut Criterion

- **Criterion: Minimum-cut**
  - Minimize weight of connections between groups

$$\arg\min_{A,B} \; cut(A,B)$$

- **Degenerate case:**



- **Problem:**
  - Only considers external cluster connections
  - Does not consider internal cluster connectivity

Graph Cut Criteria

- **Criterion:** **Normalized-cut** [Shi-Malik, '97]
  - Connectivity between groups relative to the density of each group

$$ncut(A,B) = \frac{cut(A,B)}{vol(A)} + \frac{cut(A,B)}{vol(B)}$$

: total weight of the edges with at least one endpoint in :

- **Why use this criterion?**
  - Produces more balanced partitions
- **How do we efficiently find a good partition?**
  - **Problem:** Computing optimal cut is NP-hard

Spectral Graph Partitioning

- A: adjacency matrix of undirected **G**
  - A_{ij} **=1** if is an edge, else **0**
- x is a vector in $\Re^n$ with components
  - Think of it as a label/value of each node of
- **What is the meaning of $A \cdot x$?**

$$\begin{bmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & & \vdots \\ a_{n1} & \cdots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} \qquad y_i = \sum_{j=1}^{n} A_{ij} xj = \sum_{(i,j) \in E} x_j$$

- **Entry y_i is a sum of labels x_j of neighbors of i**

What is the meaning of Ax?

- **j^{th} coordinate of $A \cdot x$:**
  - Sum of the x-values of neighbors of j
  - Make this a new value at node j
- **Spectral Graph Theory:**
  - Analyze the "spectrum" of matrix representing
  - **Spectrum:** Eigenvectors of a graph, ordered by the magnitude (strength) of their corresponding eigenvalues :

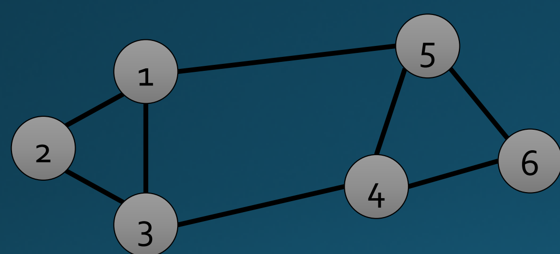
$$\begin{bmatrix} a_{11} & \dots & a_{1n} \\ \vdots & & \vdots \\ a_{n1} & \dots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} = \lambda \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}$$

$$\boldsymbol{A \cdot x = \lambda \cdot x}$$

$$\Lambda = \{\lambda_1, \lambda_2, \dots, \lambda_n\}$$
$$\lambda_1 \le \lambda_2 \le \dots \le \lambda_n$$

Matrix Representations

- **Adjacency matrix (A):**
  - $n \times n$ matrix
  - $A=[a_{ij}]$, $a_{ij}=1$ if edge between node i and j

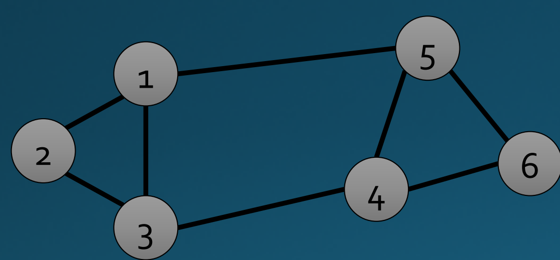


	1	2	3	4	5	6
1	0	1	1	0	1	0
2	1	0	1	0	0	0
3	1	1	0	1	0	0
4	0	0	1	0	1	1
5	1	0	0	1	0	1
6	0	0	0	1	1	0

- **Important properties:**
  - Symmetric matrix
  - Eigenvectors are real and orthogonal

Matrix Representations

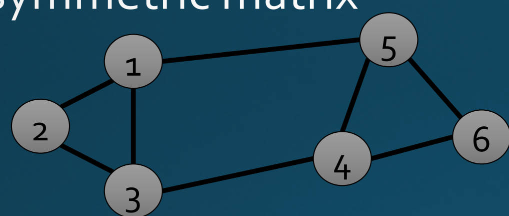
- **Degree matrix (D):**
  - $n \times n$ diagonal matrix
  - $D=[d_{ii}]$, d_{ii} = degree of node i



	1	2	3	4	5	6
1	3	0	0	0	0	0
2	0	2	0	0	0	0
3	0	0	3	0	0	0
4	0	0	0	3	0	0
5	0	0	0	0	3	0
6	0	0	0	0	0	2

Matrix Representations

- **Laplacian matrix (L):**
  - $n \times n$ symmetric matrix



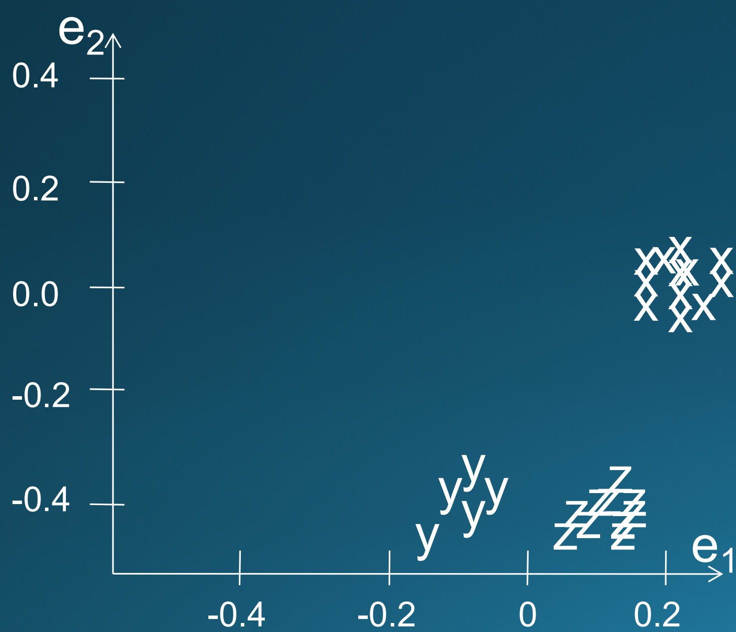
	1	2	3	4	5	6
1	3	-1	-1	0	-1	0
2	-1	2	-1	0	0	0
3	-1	-1	3	-1	0	0
4	0	0	-1	3	-1	-1
5	-1	0	0	-1	3	-1
6	0	0	0	-1	-1	2

$$L = D - A$$

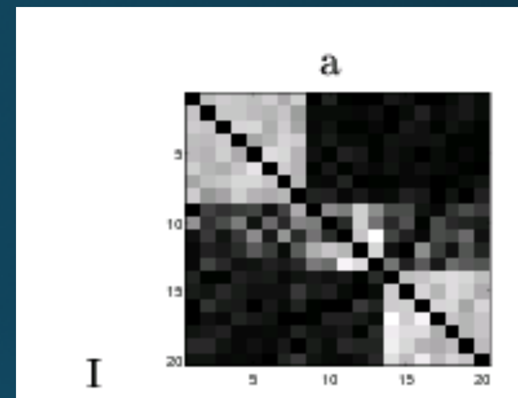
- **What is trivial eigenpair?**
- **Important properties:**
  - **Eigenvalues** are non-negative real numbers
  - **Eigenvectors** are real and orthogonal

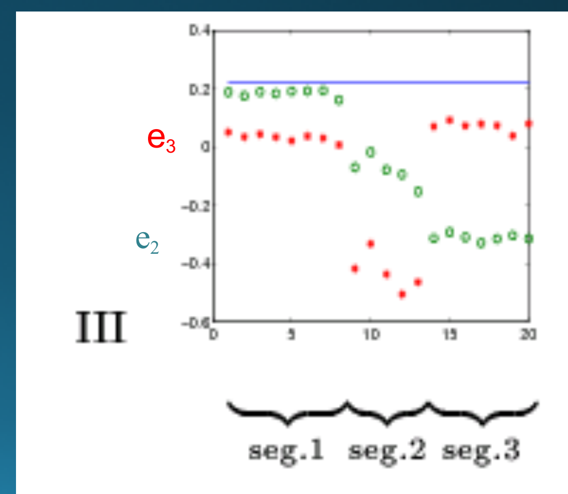
Spectral Clustering

- Graph = Matrix
  - $W * v_1 = v_2$ "propogates weights from neighbors"



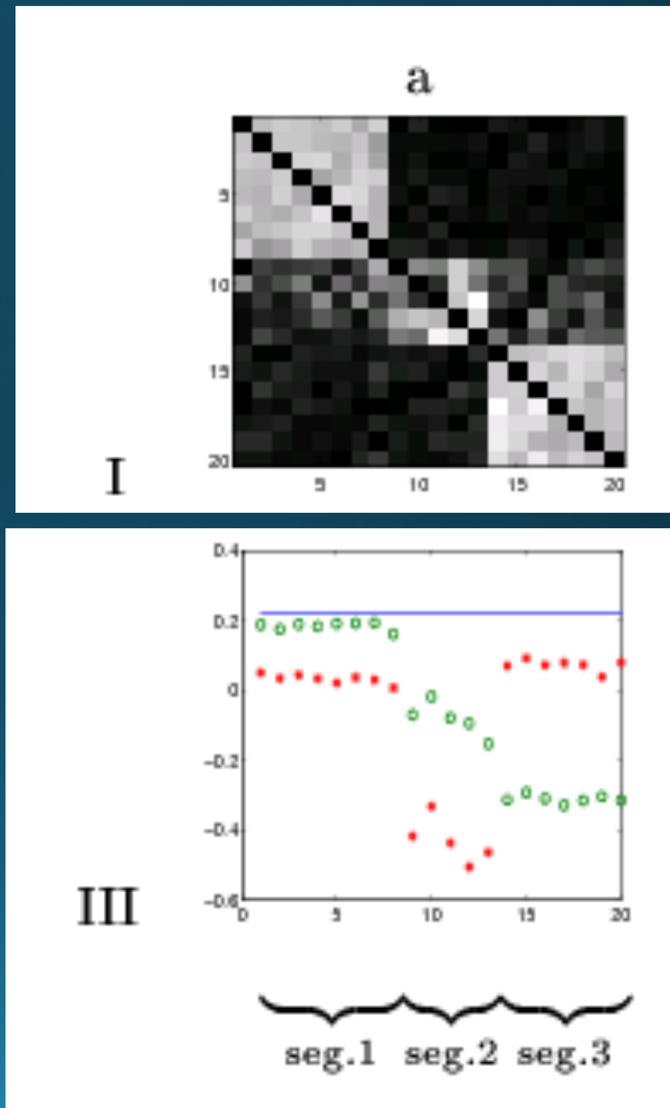
[Shi & Meila, 2002]





Spectral Clustering

- If W is connected but roughly block diagonal with k blocks, then
- the top eigenvector is a constant vector
- the next k eigenvectors are roughly piecewise constant with "pieces" corresponding to blocks

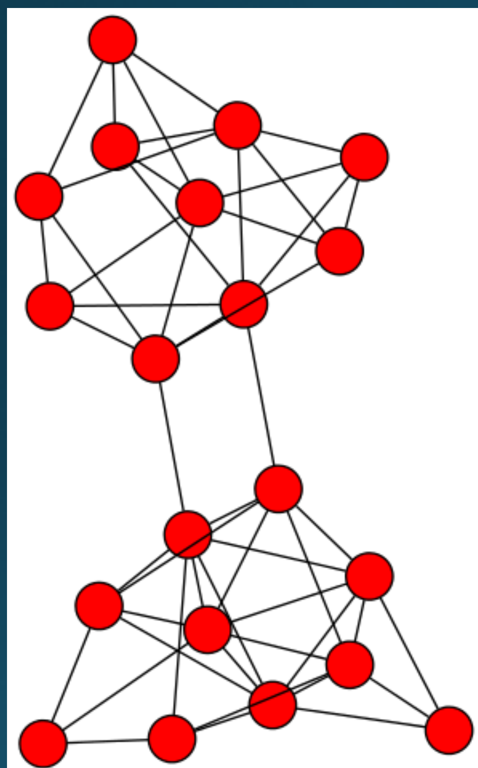


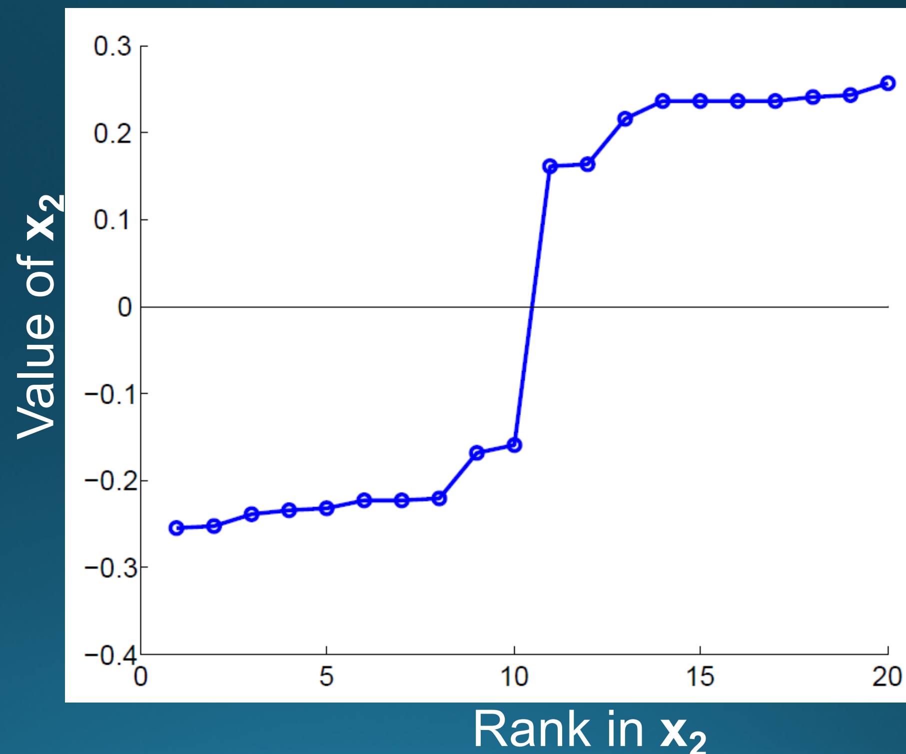
Spectral Clustering

- Outline of the algorithm:

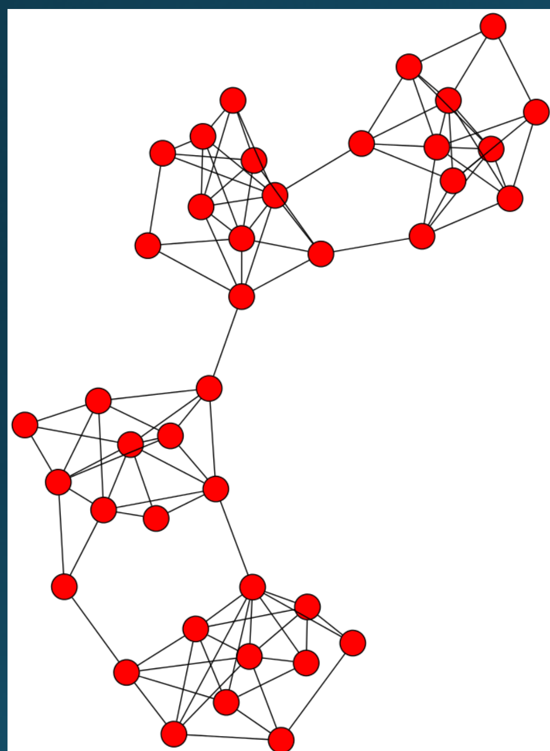
1. Find the top $k+1$ eigenvectors $\mathbf{v}_1,\ldots,\mathbf{v}_{k+1}$
2. Discard the "top" one (the "trivial pair")
3. Replace every node a with k-dimensional vector $x_a = <\mathbf{v}_2(a),\ldots,\mathbf{v}_{k+1}(a)$
4. Cluster with k-means

Example: Spectral Partitioning





Example: Spectral Partitioning



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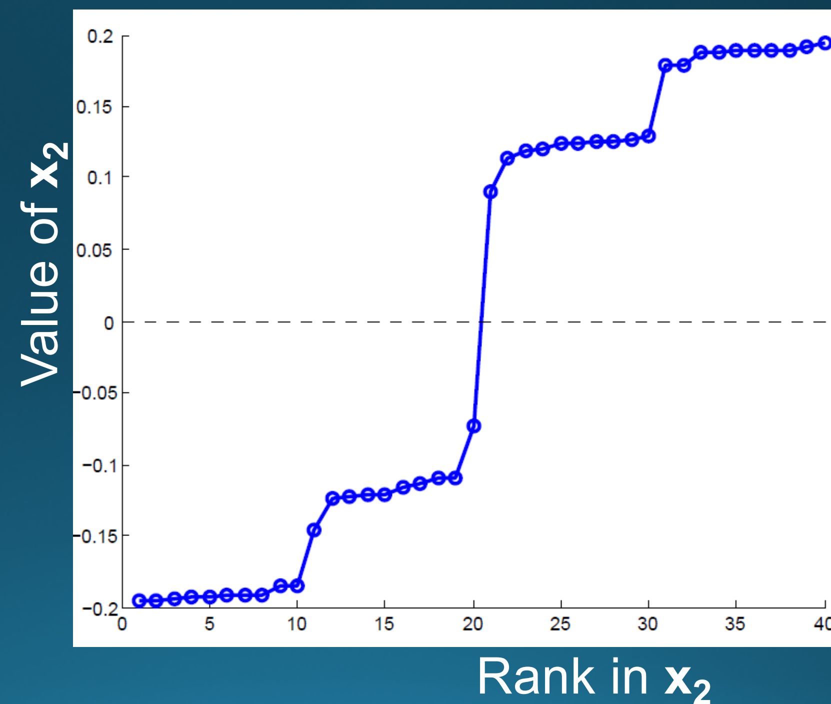
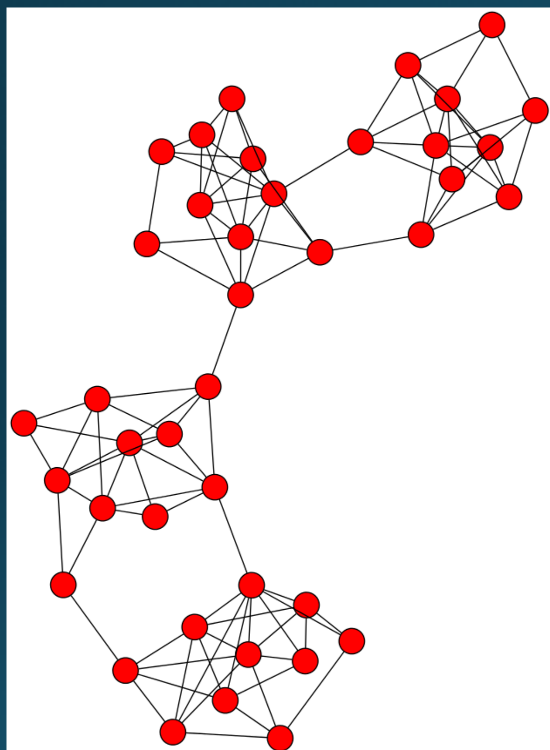
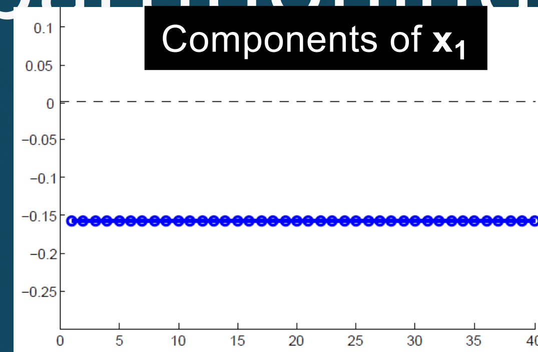
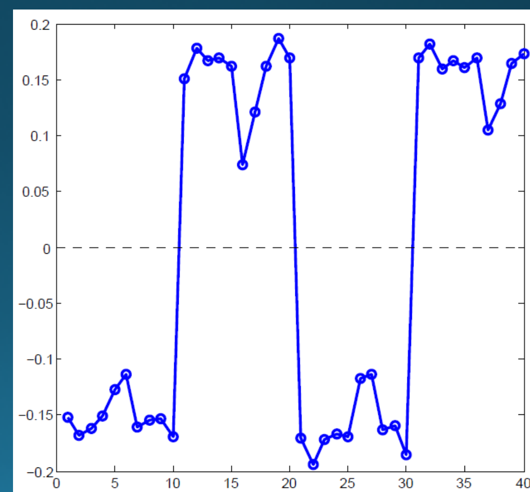


Example: Spectral partitioning







Components of x_3

k-Way Spectral Clustering

- **How do we partition a graph into k clusters?**

- **Two basic approaches:**
  - **Recursive bi-partitioning** [Hagen et al., '92]
    - Recursively apply bi-partitioning algorithm in a hierarchical divisive manner
    - Disadvantages: Inefficient, unstable
  - **Cluster multiple eigenvectors** [Shi-Malik, '00]
    - Build a reduced space from multiple eigenvectors
    - Commonly used in recent papers
    - A preferable approach…

Why use multiple eigenvectors?

- **Approximates the optimal cut** [Shi-Malik, '00]
  - Can be used to approximate optimal k-way normalized cut
- **Emphasizes cohesive clusters**
  - Increases the unevenness in the distribution of the data
  - Associations between similar points are amplified, associations between dissimilar points are attenuated
  - The data begins to "approximate a clustering"
- **Well-separated space**
  - Transforms data to a new "embedded space", consisting of k orthogonal basis vectors
- Multiple eigenvectors prevent instability due to information loss

More terms

- If A is an adjacency matrix (maybe weighted) and D is a (diagonal) matrix giving the degree of each node
- Then $L_u = D - A$ is the *(unnormalized) Laplacian*
  - $W=AD^{-1}$ is a *probabilistic adjacency matrix*
- $L_n = I - D^{-1/2}AD^{-1/2}$ is the *(normalized or random-walk) Laplacian*
- The largest eigenvectors of *W* correspond to the smallest eigenvectors of L_n
  - So sometimes people talk about "*bottom eigenvectors of the Laplacian*"

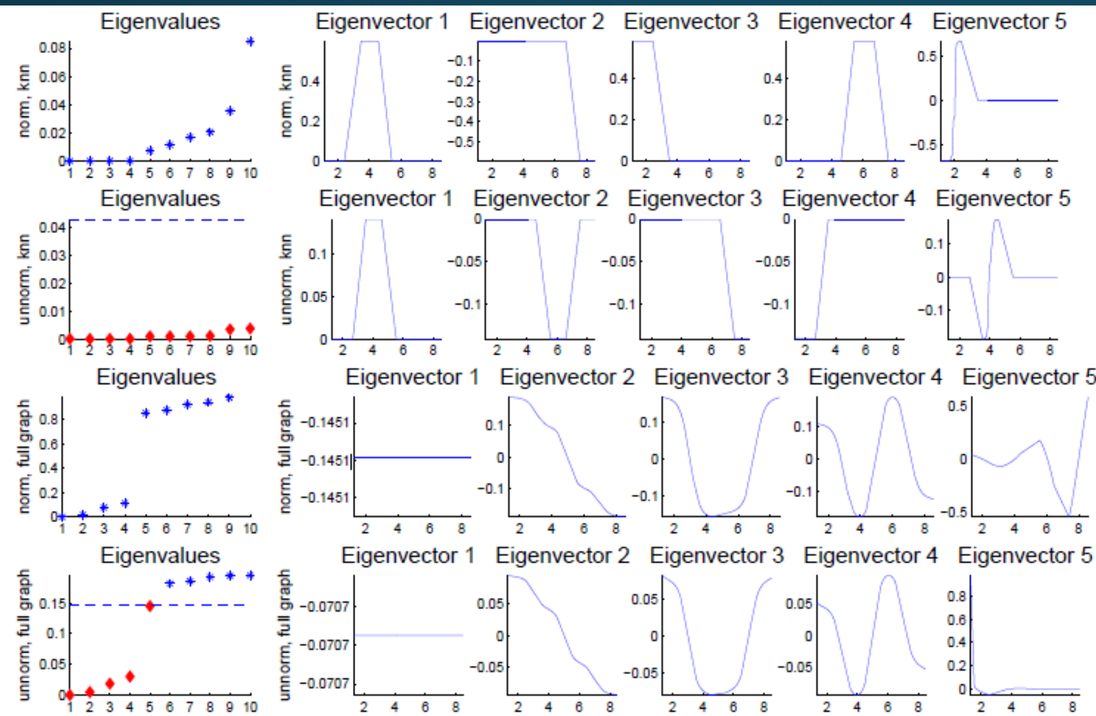


Figure 1: Toy example for spectral clustering where the data points have been drawn from a mixture of four Gaussians on $\mathbb{R}$. Left upper corner: histogram of the data. First and second row: eigenvalues and eigenvectors of L_{rw} and L based on the k-nearest neighbor graph. Third and fourth row: eigenvalues and eigenvectors of L_{rw} and L based on the fully connected graph. For all plots, we used the Gaussian kernel with $\sigma = 1$ as similarity function. See text for more details.

K-nn graph (easy)

Fully connected graph, weighted by distance

Spectrum from Data

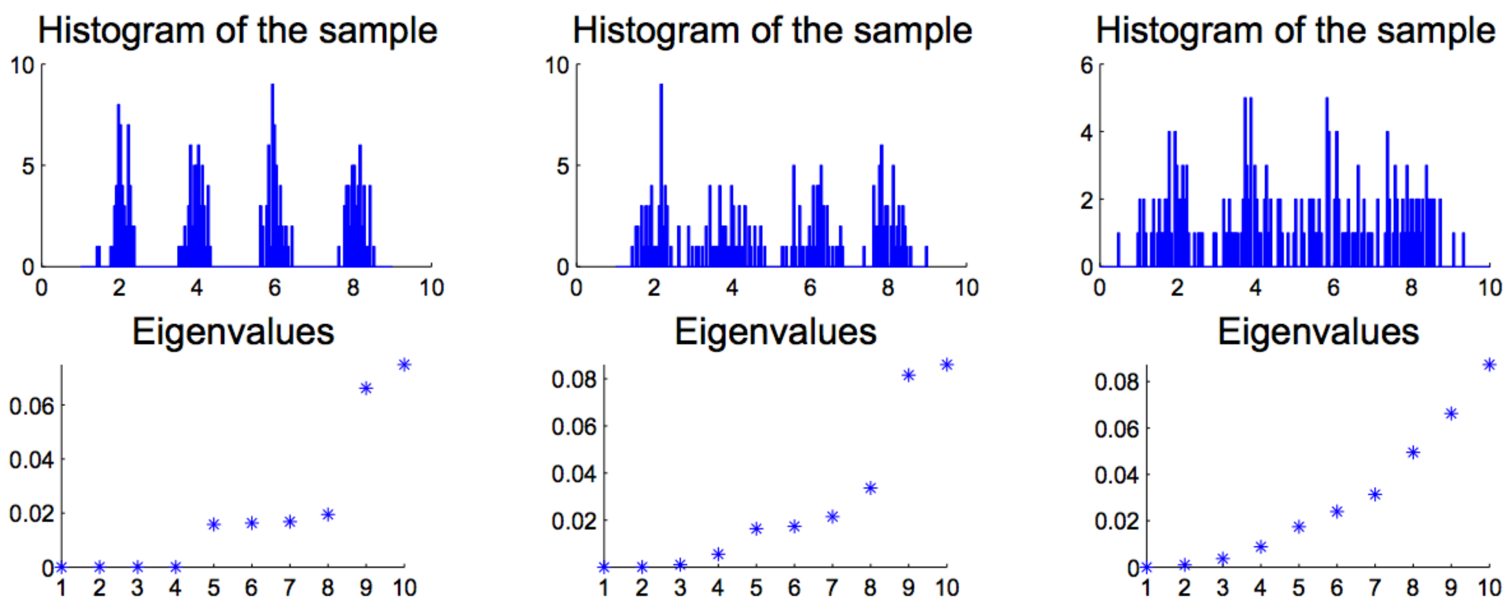
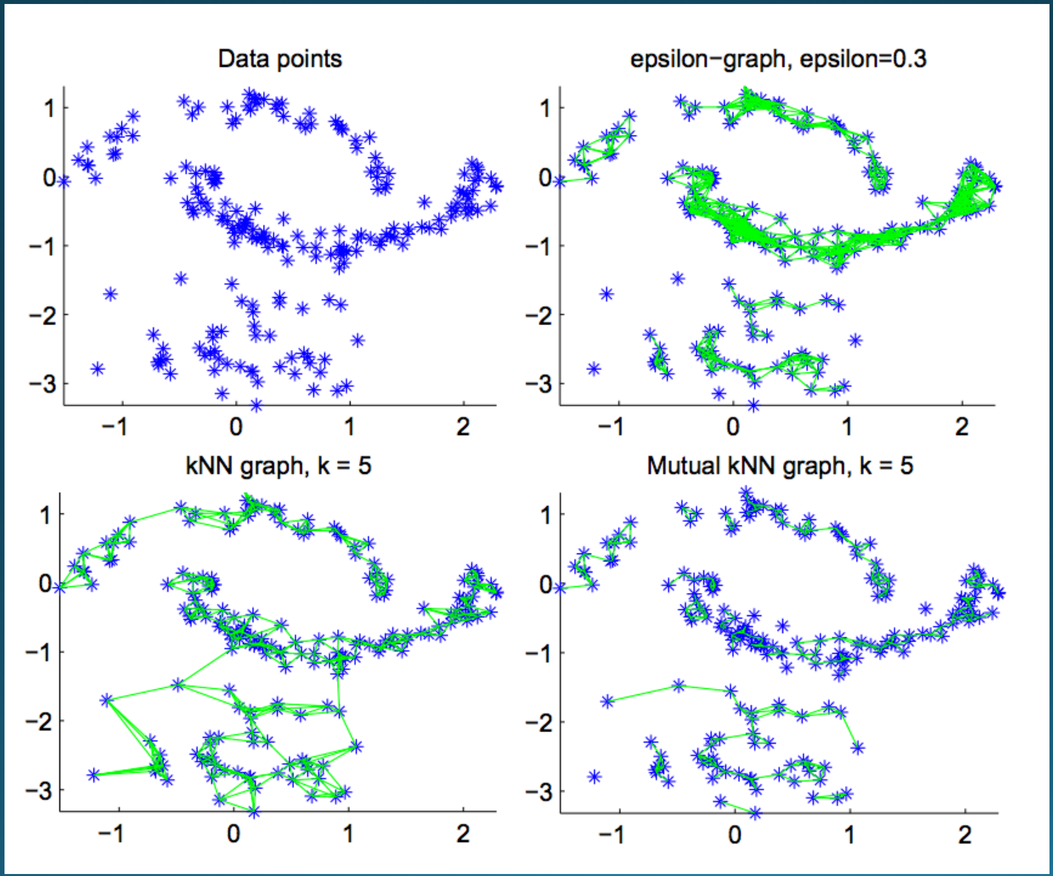


Figure 4: Three data sets, and the smallest 10 eigenvalues of L_{rw}. See text for more details.

Similarity Graphs for Spectral Clustering

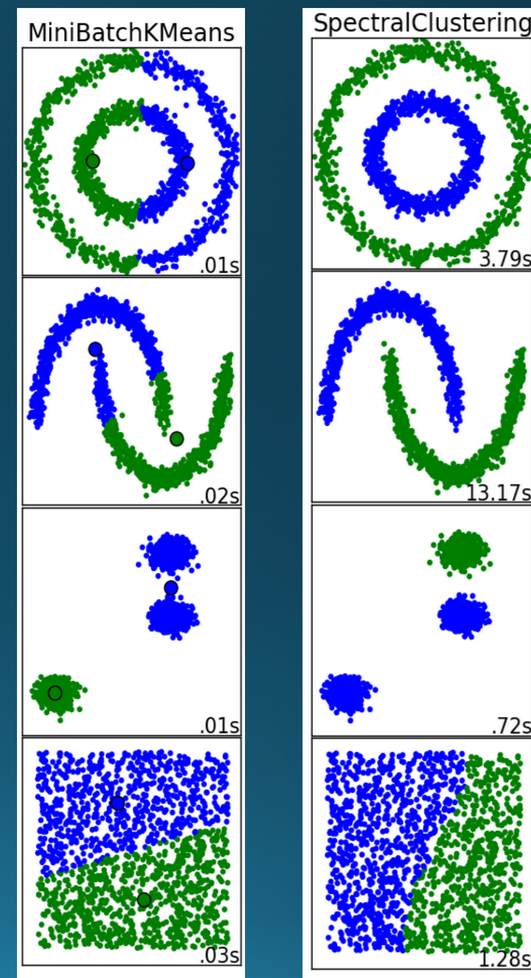


Spectral Clustering: Pros and Cons

- Elegant, and well-founded mathematically
- Works quite well when relations are approximately transitive (like similarity)
- Does not assume any form of the data (compare to K-means)
- Very noisy datasets cause problems
  - “Informative” eigenvectors need not be in top few
  - Performance can drop suddenly from good to terrible
- Expensive for very large datasets
  - Computing eigenvectors is the bottleneck

Use cases and runtimes

- K-Means
  - *Fast*
  - “Embarrassingly parallel”
  - Not very useful on anisotropic data
- Spectral clustering
  - Excellent quality under many different data forms
  - Much slower than K-Means



References

- Spectral Clustering Tutorial: http://www.informatik.uni-hamburg.de/ML/contents/people/luxburg/publications/Luxburg07_tutorial.pdf