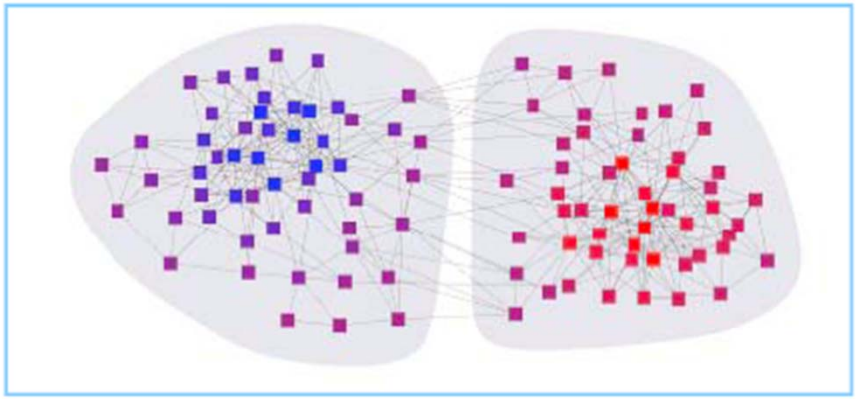
# Spectral Clustering

CS534

# Spectral Clustering

- Represent data points as the vertices V of a graph G.
- Vertices are connected by edges E
- Edges have weights *W*
  - Large weights mean that the adjacent vertices are very similar; small weights imply dissimilarity

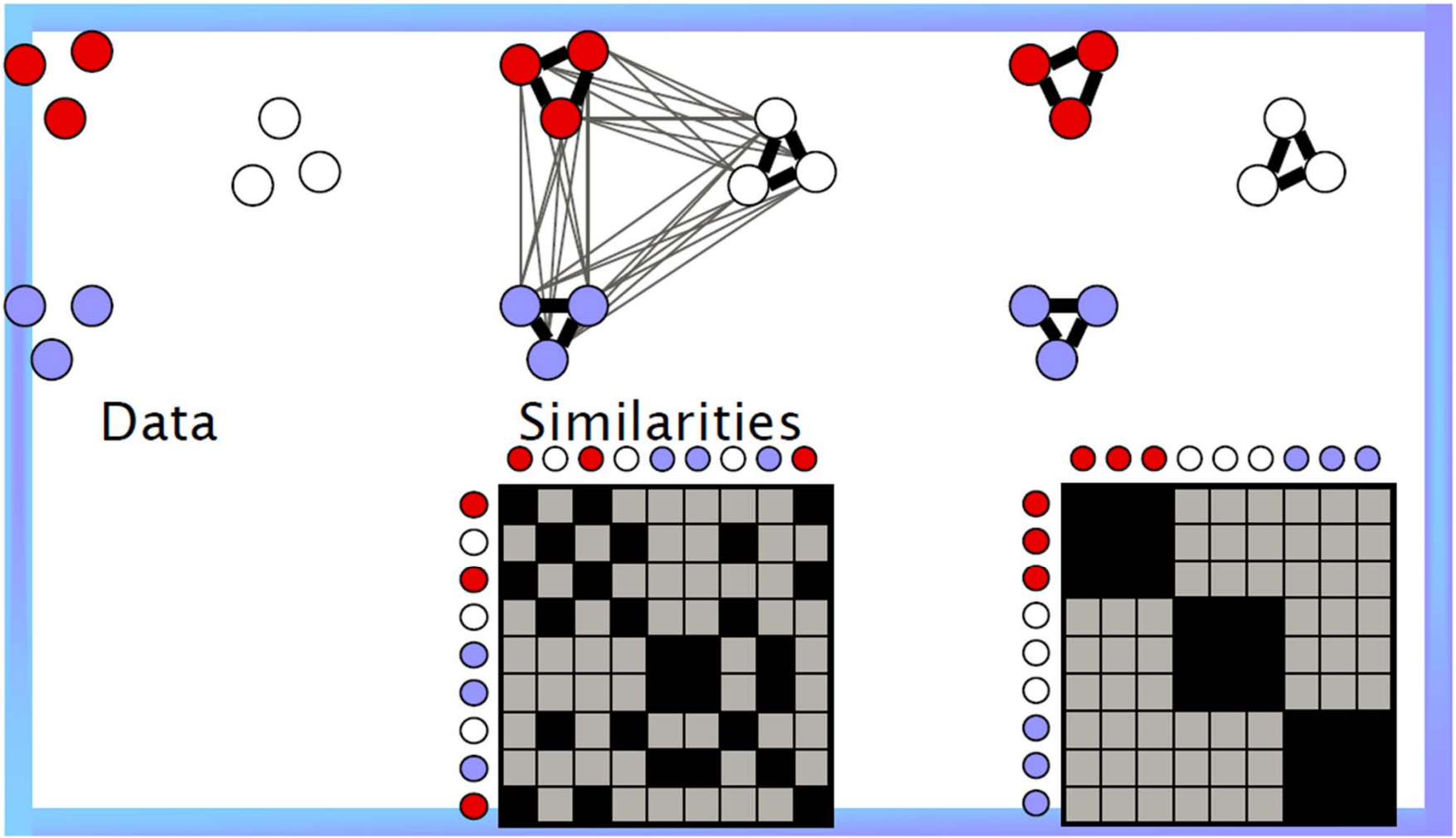


Methods that use the spectrum of the similarity matrix *W* to cluster are known as ***spectral clustering***

# Motivations/Objectives

- There are different ways to interpret the spectral clustering
- One can view spectral clustering as finding partitions of the graph that minimizes Normalized Cut
- Alternatively, we can also view this as performing a random walk on the graph

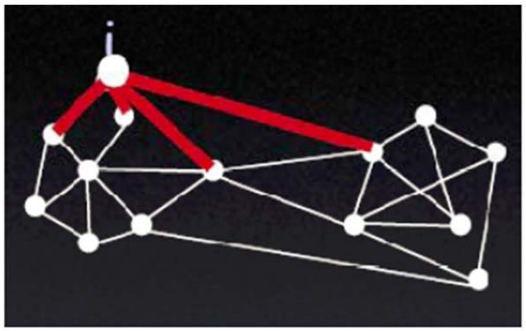
# Graph partitioning

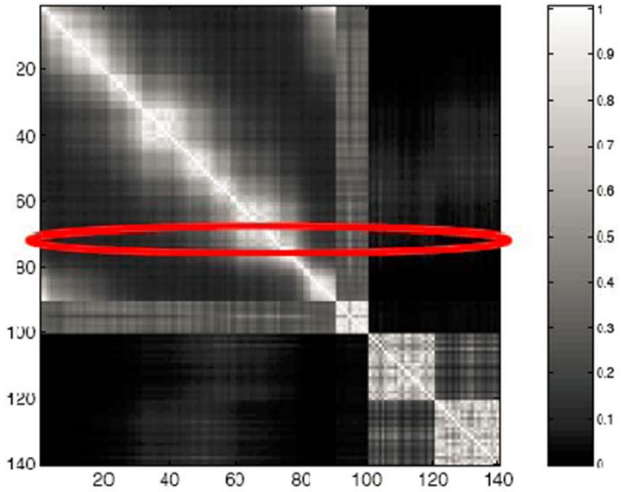


# Graph Terminologies

- Degree of nodes

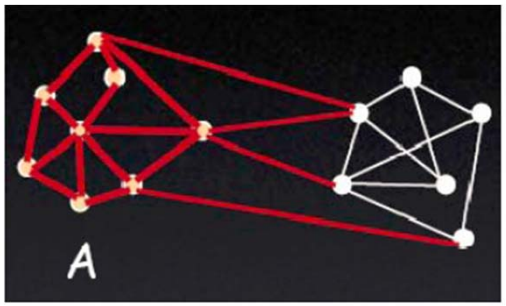
$$d_i = \sum_j w_{i,j}$$

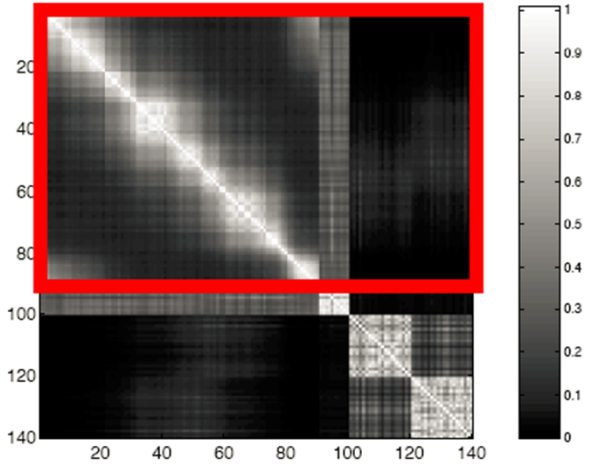



- Volume of a set

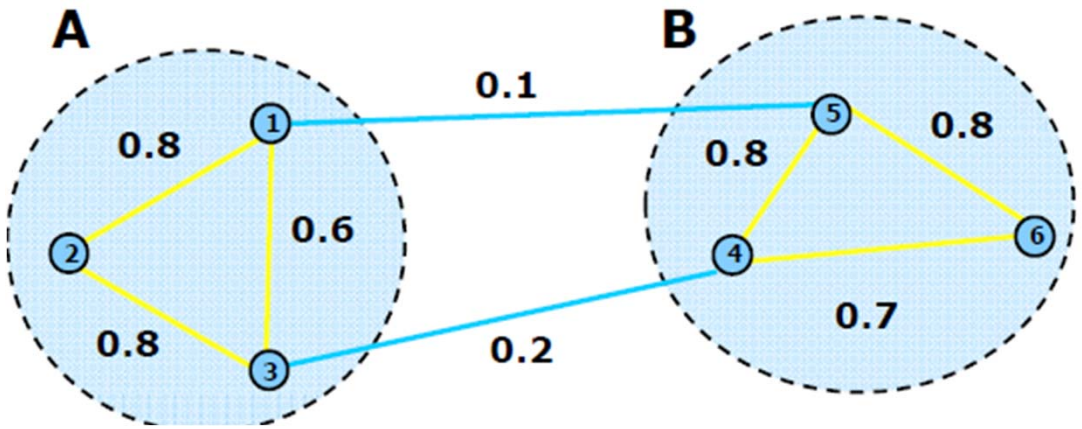
$$vol(A) = \sum_{i \in A} d_i, A \subseteq V$$



# Graph Cut

- Consider a partition of the graph into two parts A and B




- ***Cut(A, B)***: sum of the weights of the set of edges that connect the two groups

$$cut(A,B) = \sum_{i \in A, j \in B} w_{ij} = \mathbf{0.3}$$

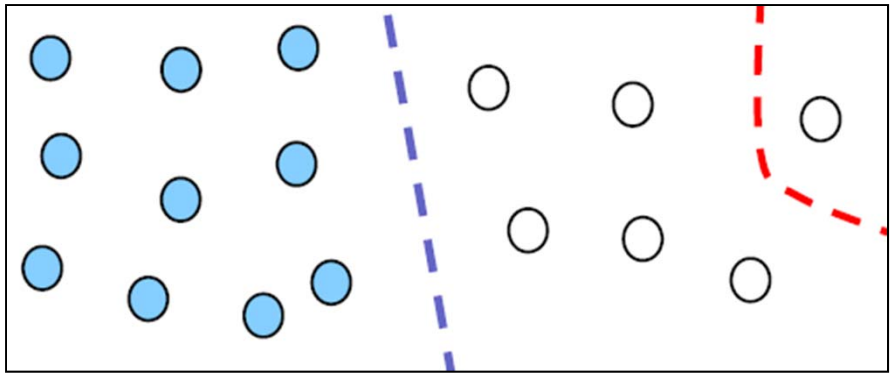
- An intuitive goal is find the partition that minimizes the cut

# Min Cut Objective

- **Mincut:** Minimize weight of connections between groups

$$\min_{A \cap B = \emptyset, A \cup B = V} Cut(A, B)$$

- Problem:
  - Prefer degenerate solution (e.g. the red partition)

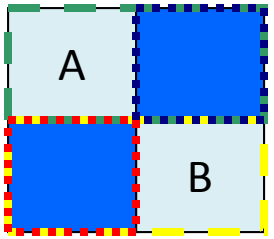


  - Need to express preference for more balanced solution

# Normalized Cut

- Consider the connectivity between groups relative to the volume of each group

$$Ncut(A,B) = \frac{cut(A,B)}{Vol(A)} + \frac{cut(A,B)}{Vol(B)}$$




$$Ncut(A,B) = cut(A,B)\frac{Vol(A)+Vol(B)}{Vol(A)Vol(B)}$$

Minimized when Vol(A) and Vol(B) are equal.
Thus encourage balanced cut

# Solving NCut

- How to minimize $Ncut$?

  Let $W$ be the similarity matrix, $W(i, j) = W_{i,j}$;
  Let D be the diag. matrix, $D(i,i) = \sum_j W(i, j)$;
  Let $x$ be a vector in $\{1,-1\}^N$, $x(i) = 1 \Leftrightarrow i \in A$.

- With some simplifications, we can show:

$$\min_x Ncut(x) = \min_y \frac{y^T(D-W)y}{y^T Dy}$$

*Rayleigh quotient*

Subject to: $y^T D1 = 0$ (***y*** *takes discrete values*)

**NP-Hard!**

# Solving NCut

- Relax the optimization problem into the continuous domain by solving generalized eigenvalue system:

$$\min_y y^T(D-W)y \text{ subject to } y^T D y = 1$$

- Which gives: $(D-W)y = \lambda D y$
- Note that $(D-W)1 = 0$, so the first eigenvector is $y_0 = 1$ with eigenvalue $0$.
- The second smallest eigenvector is the real valued solution to this problem!!

# 2-way Normalized Cuts

1. Compute the affinity matrix W, compute the degree matrix (D), D is diagonal and $D(i,i) = \sum_{j \in V} W(i,j)$
2. Solve $(D - W)y = \lambda D y$, where $D - W$ is called the Laplacian matrix
3. Use the eigenvector with the second smallest eigen-value to bipartition the graph into two parts.

# How to Create the Graph ?

- It is common to use a Gaussian Kernel to compute similarity between objects

$$W(i,j) = \exp \frac{-\left|x_i - x_j\right|^2}{\sigma^2}$$

- One could create
  - A fully connected graph
  - K-nearest neighbor graph (each node is only connected to its K-nearest neighbors)

# Creating Bi-partition Using 2nd Eigenvector

- Sometimes there is not a clear threshold to split based on the second vector since it takes continuous values
- How to choose the splitting point?
  a) Pick a constant value (0, or 0.5).
  b) Pick the median value as splitting point.
  c) Look for the splitting point that has the minimum $Ncut$ value:
     1. Choose $n$ possible splitting points.
     2. Compute $Ncut$ value.
     3. Pick minimum.

# K-way Partition?

- Recursive bi-partitioning (Hagen et al.,'91)
  - Recursively apply bi-partitioning algorithm in a hierarchical divisive manner.
  - Disadvantages: Inefficient, unstable
- Cluster multiple eigenvectors
  - Build a reduced space from multiple eigenvectors.
  - Commonly used in recent papers
  - A preferable approach… its like doing dimension reduction then k-means

# A Random Walk View of Spectral Clustering

- Imagine a random walk from node i on the graph
- Assume that the probability of taking step from node i to node j is given by the transition matrix P: $p_{ij} = \frac{W_{ij}}{D(i,i)}$
- Starting within one cluster and take a random walk governed by P, we will be likely remain in the same cluster for a long time

# Property of Random Walk

- If we start at $i_0$, where will we end up after t steps?

$$
\begin{aligned}
i_1 &\sim P_{i_0 i_1}\,, \\
i_2 &\sim \sum_{i_1} P_{i_0 i_1} P_{i_1 i_2} = \left(\mathbf{P}^2\right)_{i_0 i_2} \\
i_3 &\sim \sum_{i_2} \left(\mathbf{P}^2\right)_{i_0 i_2} P_{i_2 i_3} = \left(\mathbf{P}^3\right)_{i_0 i_3}\,, \\
&\cdots \\
i_t &\sim \left(\mathbf{P}^t\right)_{i_0 i_t}
\end{aligned}
$$

# Transition Matrix Decomposition

- Recall that $P_{ij} = \frac{W_{ij}}{D(i,i)}$, thus we have: $P = D^{-1}W$
- We will focus on a symmetric variant of this matrix $D^{-\frac{1}{2}}WD^{-\frac{1}{2}}$ for now
- We can decompose it using its eigen-vectors $z_1, \cdots, z_N$, with $|\lambda_1| \geq |\lambda_2| \geq \cdots \geq |\lambda_N|$

$$D^{-\frac{1}{2}}WD^{-\frac{1}{2}} = \lambda_1 z_1 z_1^T + \cdots + \lambda_N z_N z_N^T$$

- Spectral graph theory states that under mild conditions, we have
  - $\lambda_1 = 1$, and the rest of eigen values are less than 1

# Random Walk of Infinite Steps

$$(\mathbf{D}^{-\frac{1}{2}}\mathbf{W}\mathbf{D}^{-\frac{1}{2}})^t = (\mathbf{D}^{-\frac{1}{2}}\mathbf{W}\mathbf{D}^{-\frac{1}{2}})\cdots(\mathbf{D}^{-\frac{1}{2}}\mathbf{W}\mathbf{D}^{-\frac{1}{2}}) = \mathbf{D}^{\frac{1}{2}}\mathbf{P}^t\mathbf{D}^{-\frac{1}{2}}$$

- Thus

$$\begin{aligned}\mathbf{P}^t &= \mathbf{D}^{-\frac{1}{2}}\left(\mathbf{D}^{-\frac{1}{2}}\mathbf{W}\mathbf{D}^{-\frac{1}{2}}\right)^t\mathbf{D}^{\frac{1}{2}} \\ &= \mathbf{D}^{-\frac{1}{2}}\left(\lambda_1\mathbf{z}_1\mathbf{z}_1^T + \ldots + \lambda_N\mathbf{z}_N\mathbf{z}_N^T\right)^t\mathbf{D}^{\frac{1}{2}} \\ &= \mathbf{D}^{-\frac{1}{2}}\left(\lambda_1^t\mathbf{z}_1\mathbf{z}_1^T + \ldots + \lambda_N^t\mathbf{z}_N\mathbf{z}_N^T\right)\mathbf{D}^{\frac{1}{2}}\end{aligned}$$

- Since $\lambda_1 = 1, and\ |\lambda_i| < 1$, when $t \to \infty$, we have:

$$\mathbf{P}^\infty = \mathbf{D}^{-\frac{1}{2}}\left(\mathbf{z}_1\mathbf{z}_1^T\right)\mathbf{D}^{\frac{1}{2}}$$

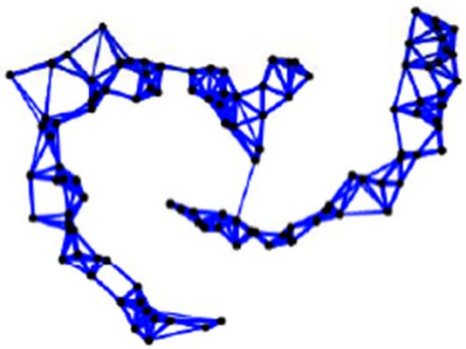
Given infinite time steps, the probability of ending in a particular node is independent of the starting node

# Finite Step Random Walk

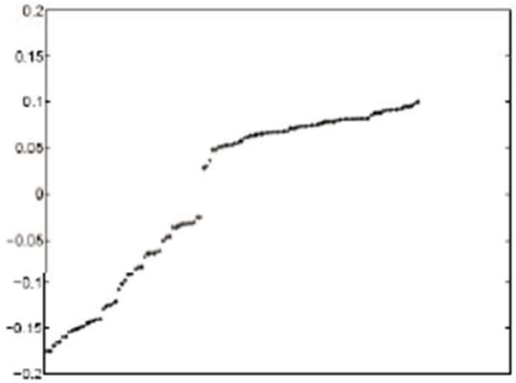
$$\mathbf{P}^t \approx \mathbf{P}^\infty + \mathbf{D}^{-\frac{1}{2}} \left(\lambda_2^2 \mathbf{z}_2 \mathbf{z}_2^T\right) \mathbf{D}^{\frac{1}{2}}$$

- Given large but finite t, we can focus on the second largest eigen-vector
- $(z_2 z_2^T)_{ij} = z_{2i} z_{2j}$, so the probability starting at $x_i$, and end up at $x_j$ is increased if $z_{2i}$ and $z_{2j}$ have the same sign
- This suggests that we should cluster based on the sign of $z_{2i}$

# Example



5–NN graph

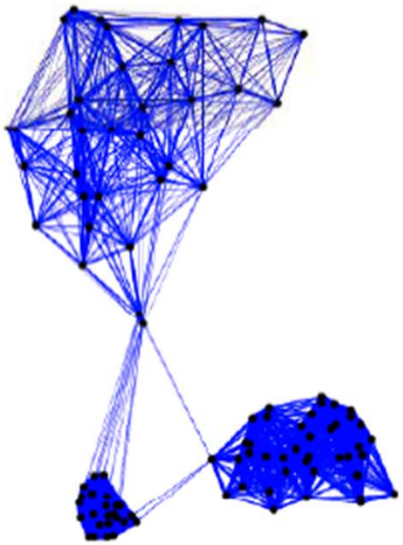



2nd eigen-vector

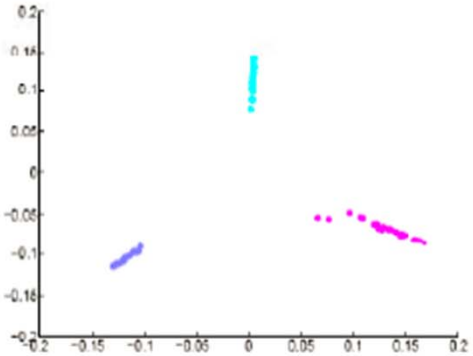
Clustering result

# Beyond bi-partition

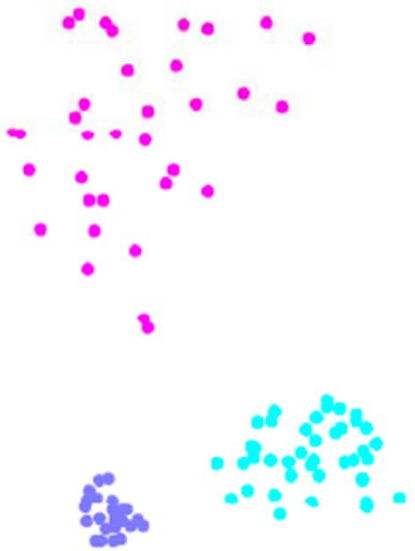
Graph, 20-NN



$\mathbf{Z}$




Clustering



# More examples, from [Ng *et al* '01]