COMPSCI 514: ALGORITHMS FOR DATA SCIENCE

Cameron Musco

University of Massachusetts Amherst. Fall 2019.

Lecture 15

Last Class:

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- Entity embeddings (e.g., word embeddings).
- Dimensionality reduction for data not lying close to a low-dimensional subspace (non-linear dimensionality reduction).
- Approach via low-rank approximation of a graph based similarity matrix (adjacency matrix).
- Spectral graph theory, spectral clustering, graph Laplacian.

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This Class: **Finish up spectral clustering.**

- Clustering non-linearly separable data via graph eigenvectors.
- Application to the *stochastic block model* and community detection.

Goal: Partition or cluster vertices in a graph based on 'similarity'.

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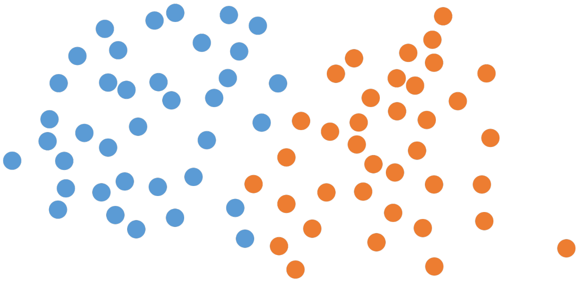
Linearly separable data.



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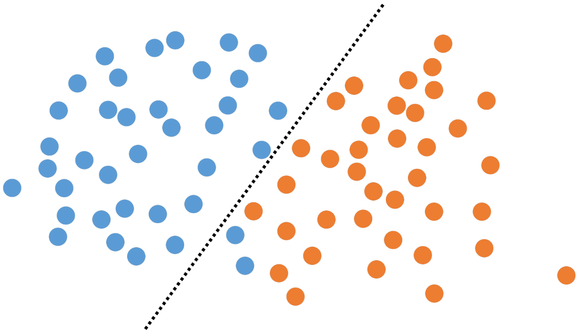

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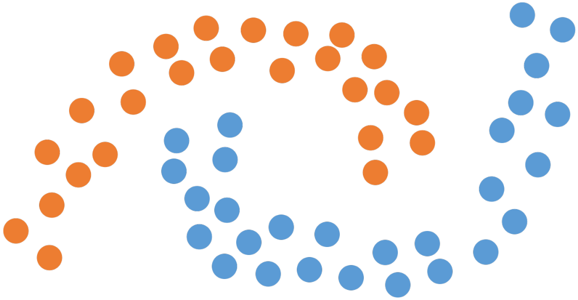
Non-linearly separable data k-nearest neighbor graph.



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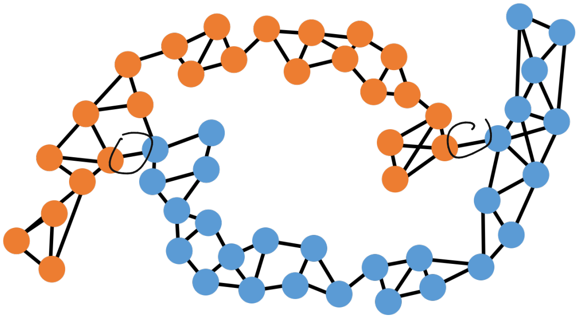

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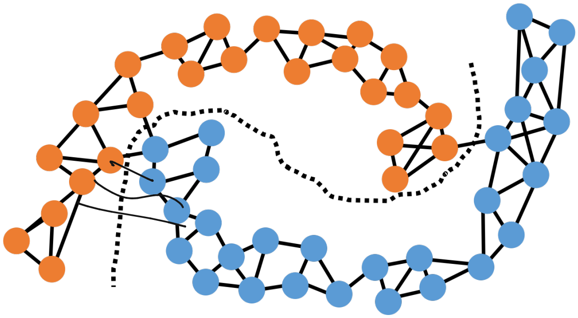

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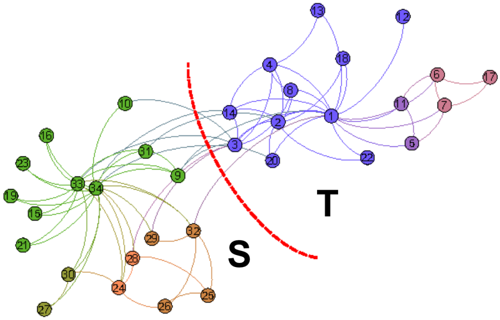
Community detection in naturally occurring networks.

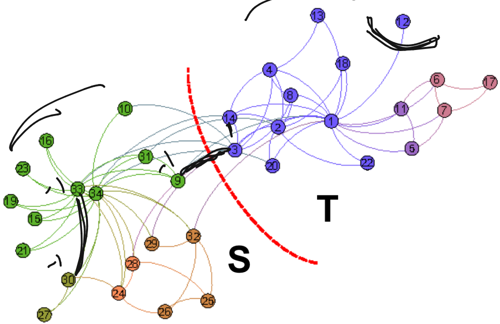


(a) Zachary Karate Club Graph

CUT MINIMIZATION

Main Idea: Partition clusters along a cut that:

1. Has few edges crossing it: $|\{(u,v) \in E : u \in S, v \in T\}|$ is small.
2. Separates large sections of the graph: $|S|, |T|$ are not too small.



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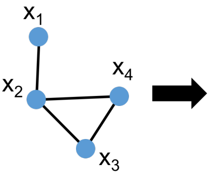
THE LAPLACIAN VIEW

For a graph with adjacency matrix **A** and degree matrix **D**, $\mathbf{L} = \mathbf{D} - \mathbf{A}$ is the graph Laplacian.



$$\mathbf{D}\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 2 \end{bmatrix} - \mathbf{A}\begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix} = \mathbf{L}\begin{bmatrix} 1 & -1 & 0 & 0 \\ -1 & 3 & -1 & -1 \\ 0 & -1 & 2 & -1 \\ 0 & -1 & -1 & 2 \end{bmatrix}$$

For a cut indicator vector $\vec{v} \in \{-1, 1\}^n$ with $\vec{v}(i) = -1$ for $i \in S$ and $\vec{v}(i) = 1$ for $i \in T$:

1. $\vec{v}^T L \vec{v} = \sum_{(i,j) \in E} (\vec{v}(i) - \vec{v}(j))^2 = 4 \cdot cut(S, T)$.
2. $\vec{v}^T \vec{1} = |T| - |S|$.

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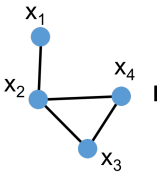

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2. $\vec{v}^T \vec{1} = |V| - |S|$.

Want to minimize both $\vec{v}^T L \vec{v}$ (cut size) and $\vec{v}^T \vec{1}$ (imbalance).

The smallest eigenvector of the Laplacian is:

$$\vec{v}_n = \frac{1}{\sqrt{n}} \cdot \vec{1} = \underset{v \in \mathbb{R}^n \text{ with } \|\vec{v}\|=1}{\arg\min} \vec{v}^T L \vec{V}$$

with $\vec{v}_n^T L \vec{v}_n = 0$.

n: number of nodes in graph, $\mathbf{A} \in \mathbb{R}^{n \times n}$: adjacency matrix, $\mathbf{D} \in \mathbb{R}^{n \times n}$: diagonal degree matrix, $\mathbf{L} \in \mathbb{R}^{n \times n}$: Laplacian matrix $\mathbf{L} = \mathbf{A} - \mathbf{D}$.

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$V_n^T D V_n - V_n^T A V_n \stackrel{?}{=} 0$

with $\vec{v}_n^T L \vec{v}_n = 0$. Why? Use that $L = D - A$.

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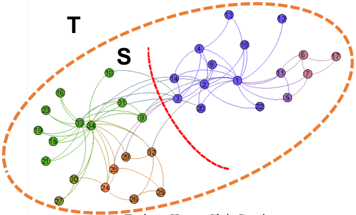

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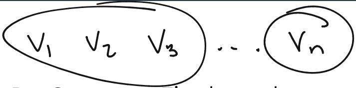
SECOND SMALLEST LAPLACIAN EIGENVECTOR



By Courant-Fischer, the second smallest eigenvector is given by:

$$\vec{v}_{n-1} = \underset{v \in \mathbb{R}^n \text{ with } \|\vec{v}\|=1,\ \vec{v}_n^T \vec{v}=0}{\arg\min} \vec{v}^T L \vec{v}$$

$= \sum \vec{v}(i) = 0$

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If $\vec{v}_{n-1}$ were in $\{-1, 1\}^n$ it would have:

- $\vec{v}_{n-1}^T L \vec{v}_{n-1} = 4 cut(S, T)$ as small as possible given that $\vec{v}_{n-1}^T \vec{1} = |T| - |S| = 0$.

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- I.e., $\vec{v}_{n-1}$ would indicate the smallest perfectly balanced cut.
- The eigenvector $\vec{v}_{n-1} \in \mathbb{R}^n$ is not generally binary, but still satisfies a 'relaxed' version of this property.

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CUTTING WITH THE SECOND LAPLACIAN EIGENVECTOR

Find a good partition of the graph by computing

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Set S to be all nodes with $\vec{v}_{n-1}(i) < 0$, T to be all with $\vec{v}_{n-1}(i) \geq 0$.

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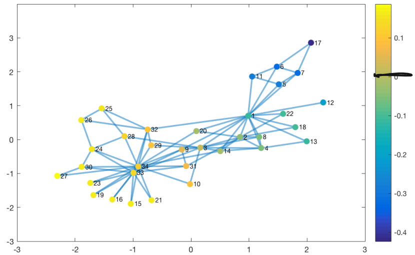

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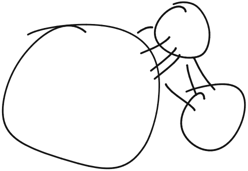

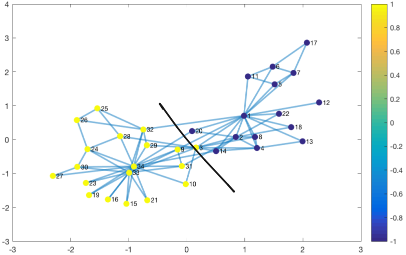

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The Shi-Malik normalized cuts algorithm is one of the most commonly used variants of this approach, using the normalized Laplacian $\bar{\mathbf{L}} = \mathbf{D}^{-1/2}\mathbf{L}\mathbf{D}^{-1/2}$.

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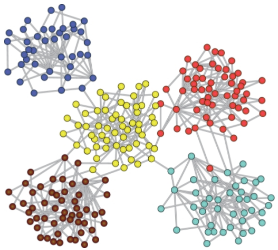
Important Consideration: What to do when we want to split the graph into more than two parts?



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Spectral Clustering:

- Compute smallest k nonzero eigenvectors $\vec{v}_{n-1}, \ldots, \vec{v}_{n-k}$ of $\bar{\mathbf{L}}$.

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Spectral Clustering: "spectral embedding"

- Compute smallest k nonzero eigenvectors $\vec{v}_{n-1}, \ldots, \vec{v}_{n-k}$ of $\overline{\mathbf{L}}$.
- Represent each node by its corresponding row in $\mathbf{V} \in \mathbb{R}^{n \times k}$ whose ~~rows~~ columns are $\vec{v}_{n-1}, \ldots \vec{v}_{n-k}$.

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- Cluster these rows using k-means clustering (or really any clustering method).

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The smallest eigenvectors of $\mathbf{L} = \mathbf{D} - \mathbf{A}$ give the orthogonal 'functions' that are smoothest over the graph. I.e., minimize

$$\vec{v}^T L \vec{v} = \sum_{(i,j) \in E} [\vec{v}(i) - \vec{v}(j)]^2.$$

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Embedding points with coordinates given by $[\vec{v}_{n-1}(j), \vec{v}_{n-2}(j), \ldots, \vec{v}_{n-k}(j)]$ ensures that coordinates connected by edges have minimum total squared Euclidean distance.

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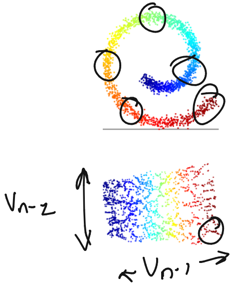

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$V_{n-1} L V_{n-1} + V_{n-2} L V_{n-2}^T \ldots$

$= \sum_{(i,j) \in E} \|x(i) - x(j)\|_2^2$

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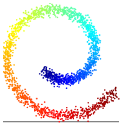
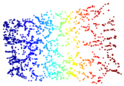
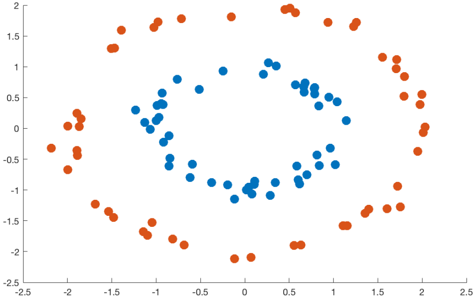


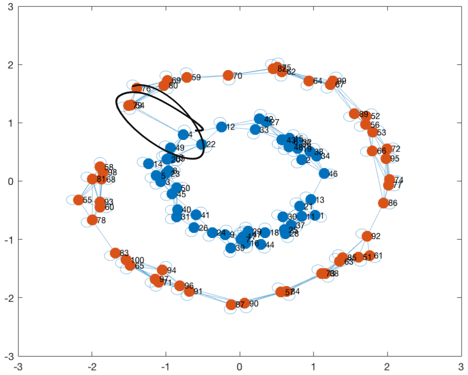


- Spectral Clustering
- Laplacian Eigenmaps
- Locally linear embedding
- Isomap
- Etc...

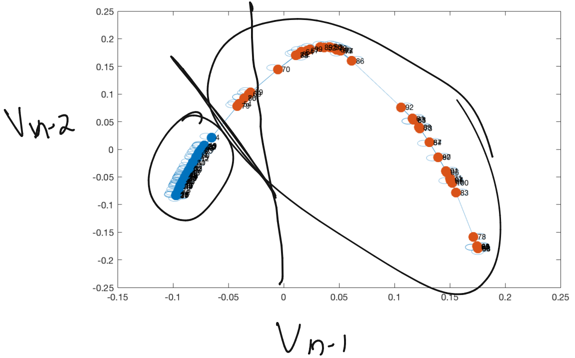
Original Data: (not linearly separable)



k-Nearest Neighbors Graph:



Embedding with eigenvectors $\vec{v}_{n-1}, \vec{v}_{n-2}$: (linearly separable)



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Common Approach: Give a natural generative model for random inputs and analyze how the algorithm performs on inputs drawn from this model.

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- Haven't given any formal guarantee on the 'quality' of the partitioning.
- This is difficult to do for general input graphs.

Common Approach: Give a natural generative model for random inputs and analyze how the algorithm performs on inputs drawn from this model.

- Very common in algorithm design for data analysis/machine learning (can be used to justify ℓ_2 linear regression, k-means clustering, PCA, etc.)

Stochastic Block Model (Planted Partition Model): Let $G_n(p, q)$ be a distribution over graphs on n nodes, split equally into two groups B and C, each with $n/2$ nodes.

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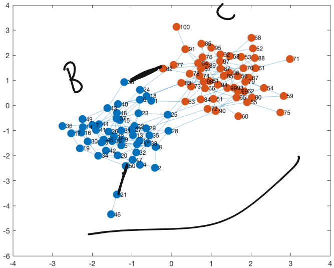

Let G be a stochastic block model graph drawn from $G_n(p, q)$.

$G_n(p, q)$: stochastic block model distribution. B, C: groups with $n/2$ nodes each. Connections are independent with probability p between nodes in the same group, and probability q between nodes not in the same group.

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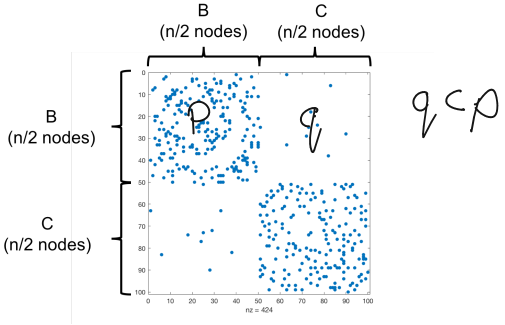

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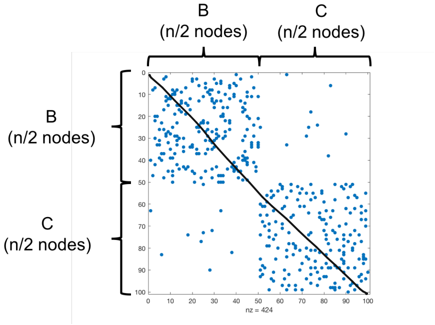

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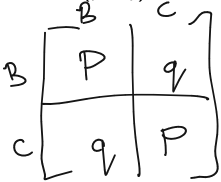
Letting G be a stochastic block model graph drawn from $G_n(p, q)$ and $\mathbf{A} \in \mathbb{R}^{n \times n}$ be its adjacency matrix. What is $\mathbb{E}[\mathbf{A}]$? $= \bar{A}$



$\bar{A}_{ij} = \mathbb{E} A_{ij} = p$ i,j in same group

$\bar{A}_{ij} = \mathbb{E} A_{ij} = q$ if i,j in diff. groups

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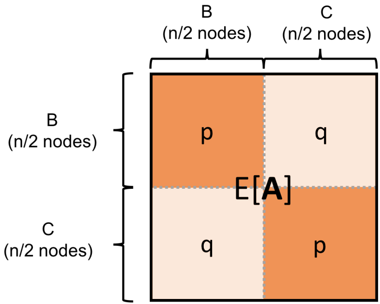
Letting G be a stochastic block model graph drawn from $G_n(p,q)$ and $\mathbf{A} \in \mathbb{R}^{n\times n}$ be its adjacency matrix. $(\mathbb{E}[\mathbf{A}])_{i,j} = p$ for i,j in same group, $(\mathbb{E}[\mathbf{A}])_{i,j} = q$ otherwise.



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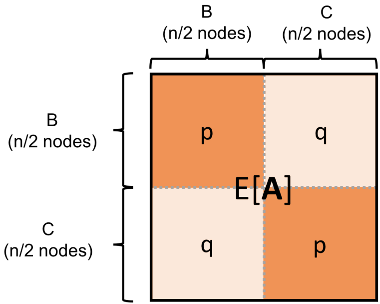

What are the eigenvectors and eigenvalues of $\mathbb{E}[\mathbf{A}]$?

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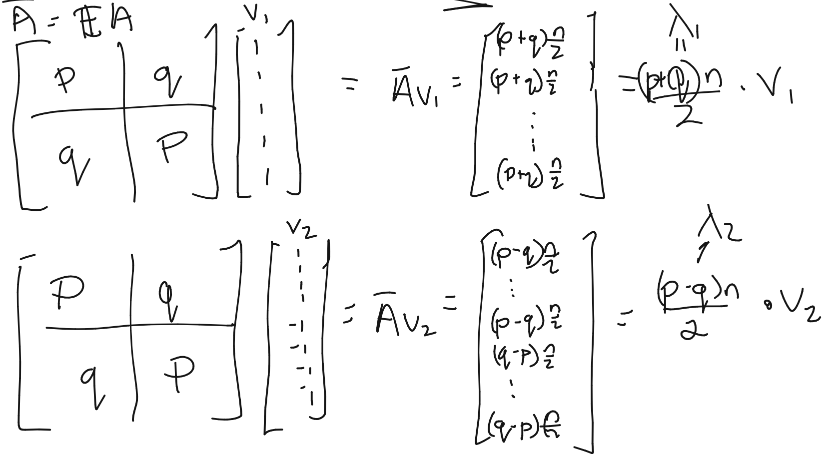

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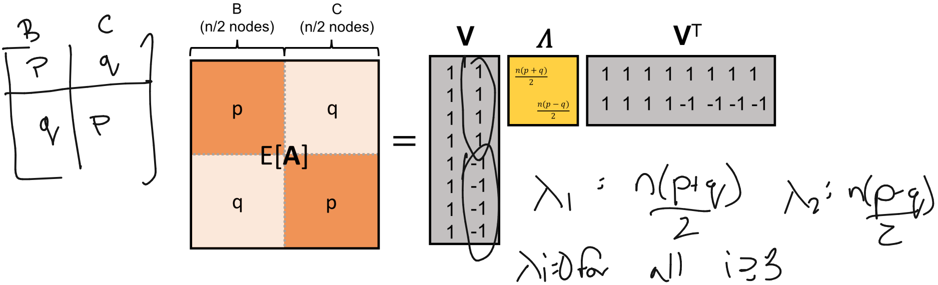
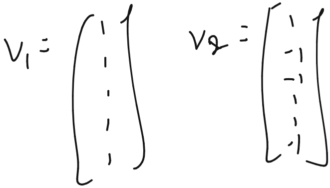
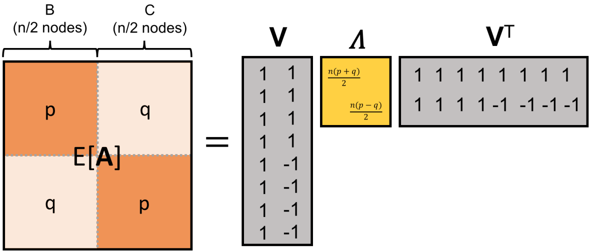
EXPECTED ADJACENCY SPECTRUM



If we compute $\vec{v}_2$ then we recover the communities *B* and *C*!





If we compute $\vec{v}_2$ then we recover the communities B and C!

- Can show that for $G \sim G_n(p, q)$, $\mathbf{A}$ is close to $\mathbb{E}[\mathbf{A}]$ with high probability.
- Thus, the true second eigenvector of A is close to $[1, 1, 1, \ldots, -1, -1, -1]$ and gives a good estimate of the communities.

Letting G be a stochastic block model graph drawn from $G_n(p, q)$, $\mathbf{A} \in \mathbb{R}^{n \times n}$ be its adjacency matrix and $\mathbf{L}$ be its Laplacian, what are the eigenvectors and eigenvalues of $\mathbb{E}[\mathbf{L}]$?

$$\mathbb{E}[L] = \mathbb{E}[D - A] = \mathbb{E}D - \left[\begin{array}{c|c} p & q \\ \hline q & p \end{array}\right]$$

$$\left[p\left(\frac{n}{2}\right) + q\left(\frac{n}{2}\right)\right] I - \left[\begin{array}{c|c} p & q \\ \hline q & p \end{array}\right]$$

$\bar{L} = \mathbb{E}L$, $\bar{A} = \mathbb{E}A$

$$\bar{L} = \frac{(p+q)n}{2} I - \bar{A}$$

v_i which is eigenvector of $\bar{A}$

$$\bar{L}v_i = \frac{(p+q)n}{2} I v_i - \bar{A}v_i = \left[\frac{(p+q)n}{2} - \lambda_i(A)\right] v_i$$

Letting G be a stochastic block model graph drawn from $G_n(p, q)$, $\mathbf{A} \in \mathbb{R}^{n \times n}$ be its adjacency matrix and $\mathbf{L}$ be its Laplacian, what are the eigenvectors and eigenvalues of $\mathbb{E}[\mathbf{L}]$?

Questions?