COMPSCI 514: ALGORITHMS FOR DATA SCIENCE

Andrew McGregor

Lecture 19

Last Class: Spectral Clustering

- Spectral clustering: finding good cuts via Laplacian eigenvectors.

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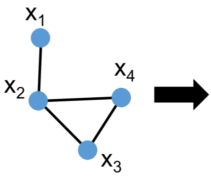
This Class: Stochastic Block Model

- Stochastic block model: A simple clustered graph model where we can prove the effectiveness of spectral clustering.
- Prove that clustering with the Laplacian eigenvectors (spectral clustering) finds communities in the stochastic block model.

REVIEW

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



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

How smooth any vector $\vec{v}$ is over the graph can be measured by:

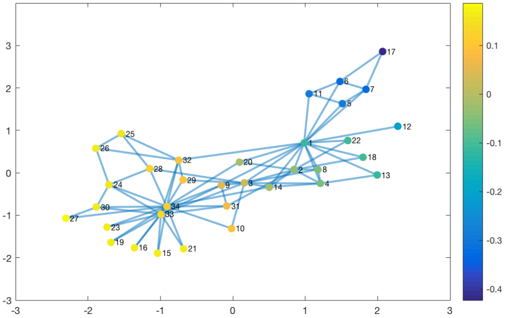
$$\sum_{(i,j)\in E} (\vec{v}(i) - \vec{v}(j))^2 = \vec{v}^T \mathbf{L} \vec{v}.$$

- We'll use eigenvectors of Laplacian to divide the nodes of the graph into roughly equal groups such that the number of cut edges is small.

Find a good partition of the graph by computing

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

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



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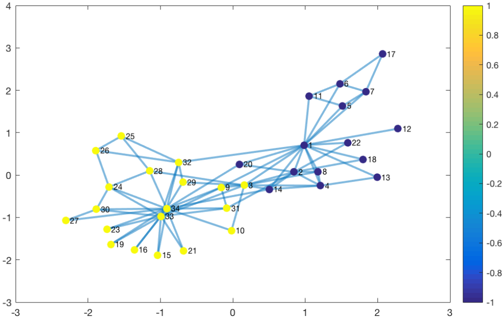

For a cut indicator vector $\vec{v} \in \{-1, 1\}^n$ with $\vec{v}(i) = -1$ for $i \in S$ and $\vec{v}(i) = 1$ for $i \in T$:

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

THE LAPLACIAN VIEW

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Next Step: See how this dual minimization problem is naturally solved by eigendecomposition.

SMALLEST LAPLACIAN EIGENVECTOR

The smallest eigenvector of the Laplacian is:

$$\vec{v}_1 = \frac{1}{\sqrt{n}} \cdot \vec{1} = \underset{v \in \mathbb{R}^n \text{ with } \|\vec{v}\|=1}{\arg\min} \vec{v}^T L \vec{v}$$

with eigenvalue $\vec{v}_1^T L \vec{v}_1 = 0$.

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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SECOND SMALLEST LAPLACIAN EIGENVECTOR

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

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If $\vec{v}_2$ were in $\left\{-\frac{1}{\sqrt{n}}, \frac{1}{\sqrt{n}}\right\}^n$ it would have:

- $\vec{v}_2^T L \vec{v}_2 = \frac{4}{n} \cdot cut(S, T)$ as small as possible subject to

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- I.e., $\vec{v}_2$ would indicate the smallest perfectly balanced cut.
- The eigenvector $\vec{v}_2 \in \mathbb{R}^n$ is not generally binary, but still satisfies a 'relaxed' version of this property.

CUTTING WITH THE SECOND LAPLACIAN EIGENVECTOR

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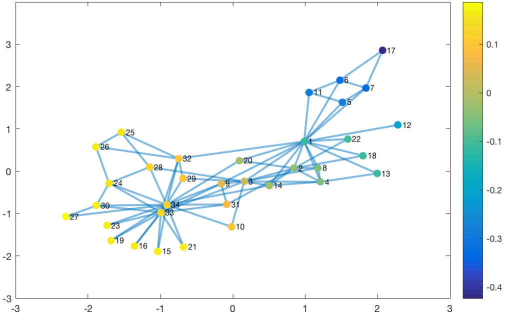

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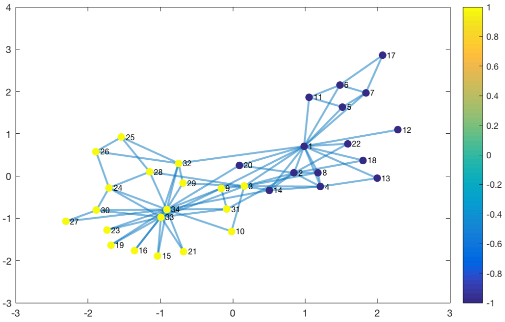

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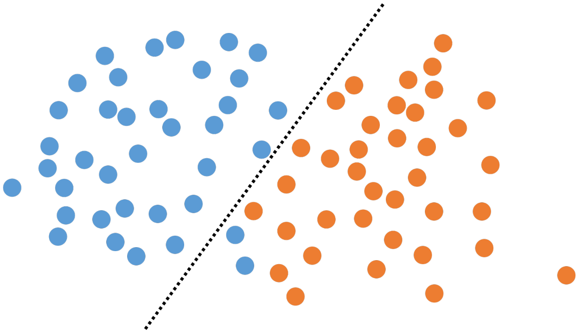

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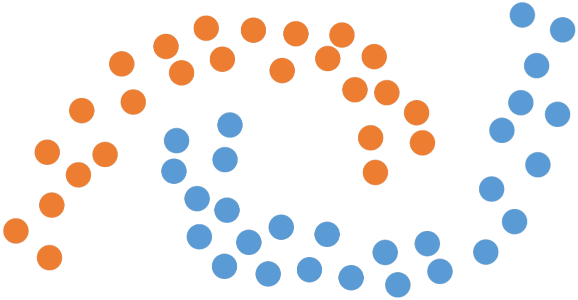
Non-linearly separable data k-nearest neighbor graph.



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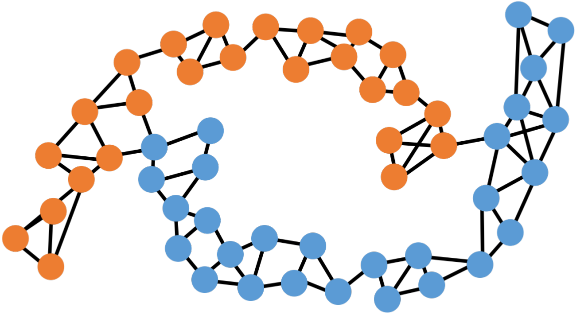

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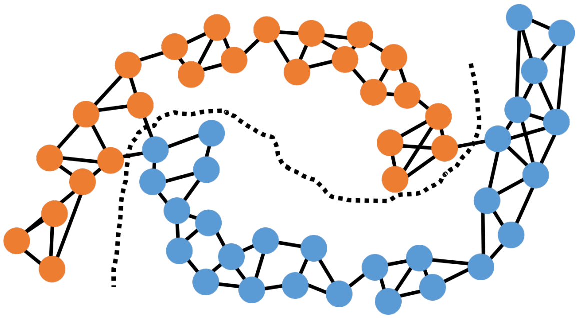

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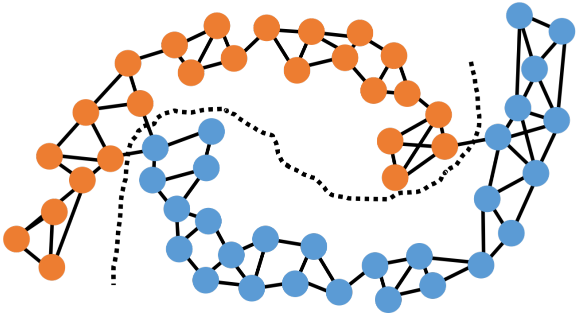

Can find this cut using eigendecomposition!

SPECTRAL PARTITIONING IN PRACTICE

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

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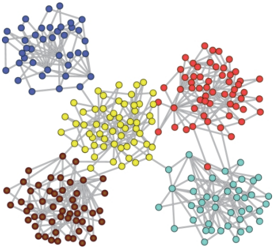

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- Compute smallest t nonzero eigenvectors $\vec{v}_2, \ldots, \vec{v}_{t+1}$ of $\overline{\mathbf{L}}$.

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- Represent each node by its corresponding row in $\mathbf{V} \in \mathbb{R}^{n \times t}$ whose columns are $\vec{v}_2, \ldots \vec{v}_{t+1}$.

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

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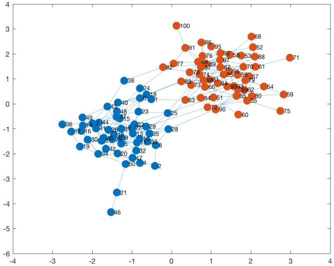
Common Approach: Give a natural generative model for random inputs and analyze how the algorithm performs on inputs drawn from this model.

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

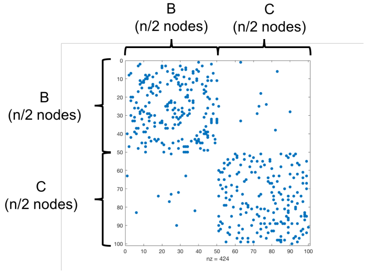
Stochastic Block Model (Planted Partition Model): Let $G_n(p, q)$ be a distribution over graphs on n nodes, split randomly into two groups B and C, each with $n/2$ nodes.

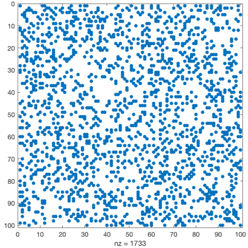
- Any two nodes in the same group are connected with probability p (including self-loops).
- Any two nodes in different groups are connected with prob. $q < p$.
- Connections are independent.



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

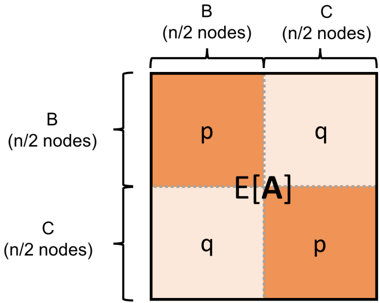
- Let $\mathbf{A} \in \mathbb{R}^{n \times n}$ be the adjacency matrix of G, ordered in terms of group ID.





$G_n(p, q)$: 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.

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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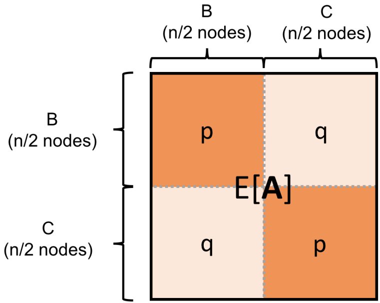

What is rank($\mathbb{E}[\mathbf{A}]$)?
What are the eigenvectors and eigenvalues of $\mathbb{E}[\mathbf{A}]$?

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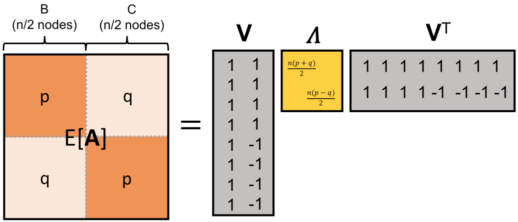
EXPECTED ADJACENCY SPECTRUM



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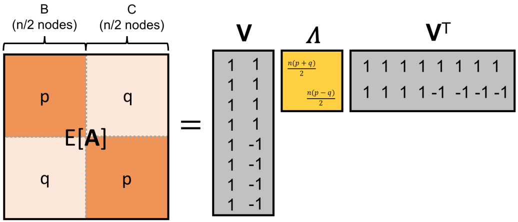

If we compute $\vec{v}_2$ then we recover the communities B and C!

- Can show that for $G \sim G_n(p,q)$, $\mathbf{A}$ is "close" to $\mathbb{E}[\mathbf{A}]$ in some appropriate sense (matrix concentration inequality).
- Second eigenvector of A is close to $[1,1,1,\ldots,-1,-1,-1]$ and gives a good estimate of the communities.

When the rows/columns aren't sorted by community ID, the second eigenvector is something like $[1,-1,1,-1,\ldots,1,1,-1]$ and the entries give community ids.