COMPSCI 514: ALGORITHMS FOR DATA SCIENCE

Andrew McGregor

Lecture 18

SUMMARY

This Class: Spectral Clustering

- Finding good cuts via Laplacian eigenvectors.
- Start analysis via the stochastic block model.

GRAPH CLUSTERING

SPECTRAL CLUSTERING

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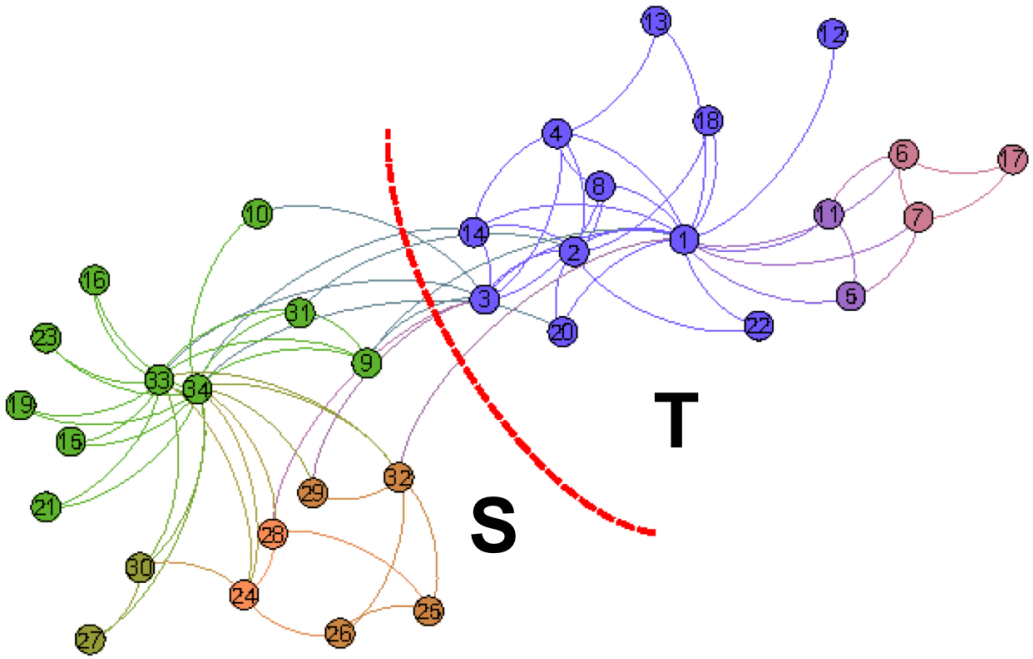
Community detection in naturally occurring networks.



(a) Zachary Karate Club Graph

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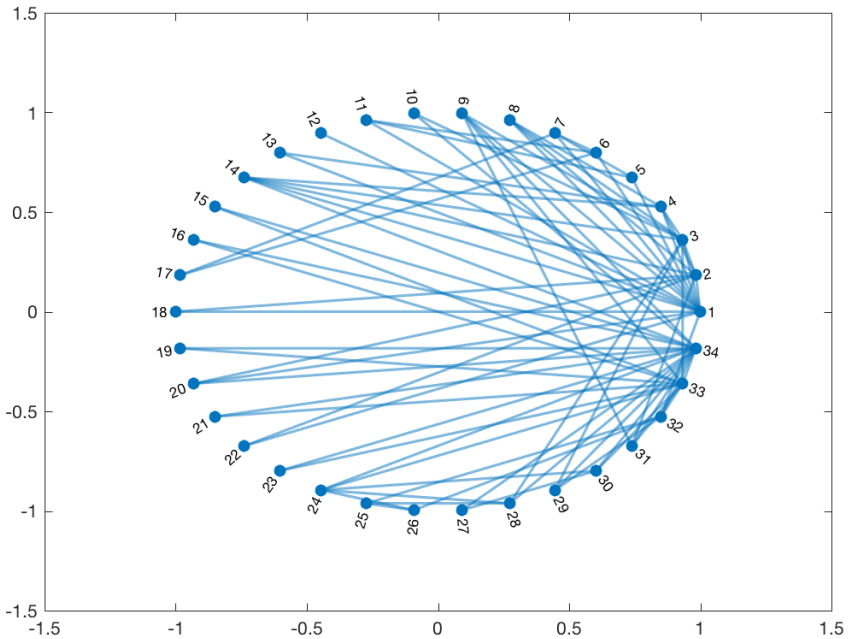

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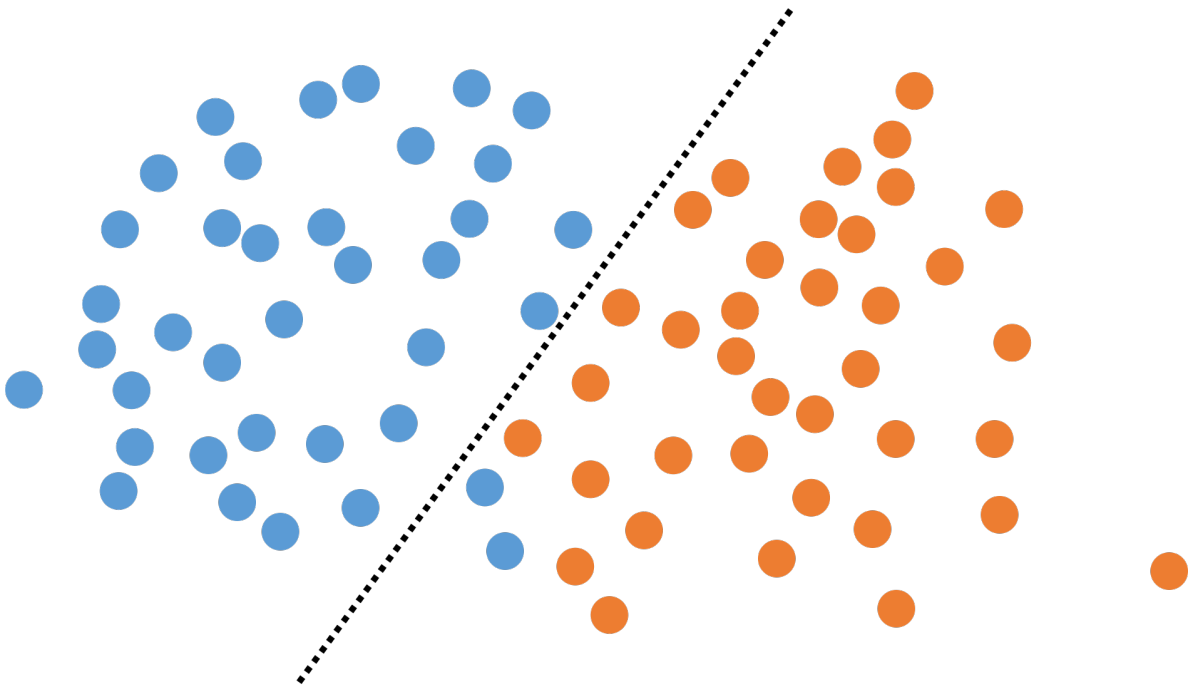
Linearly separable data.



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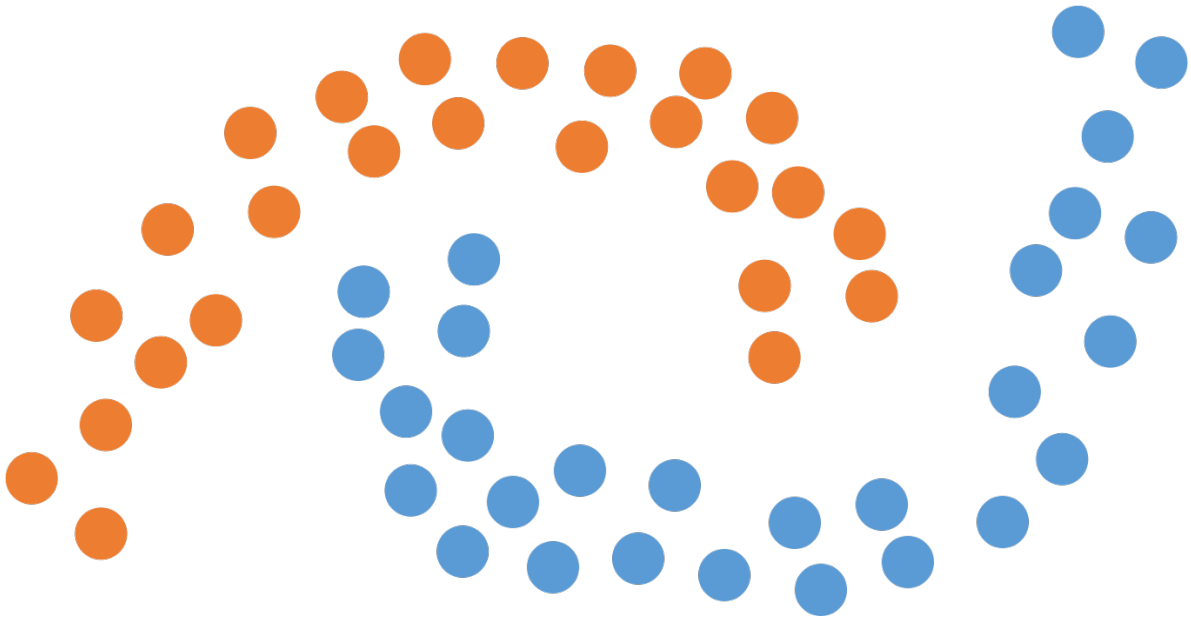

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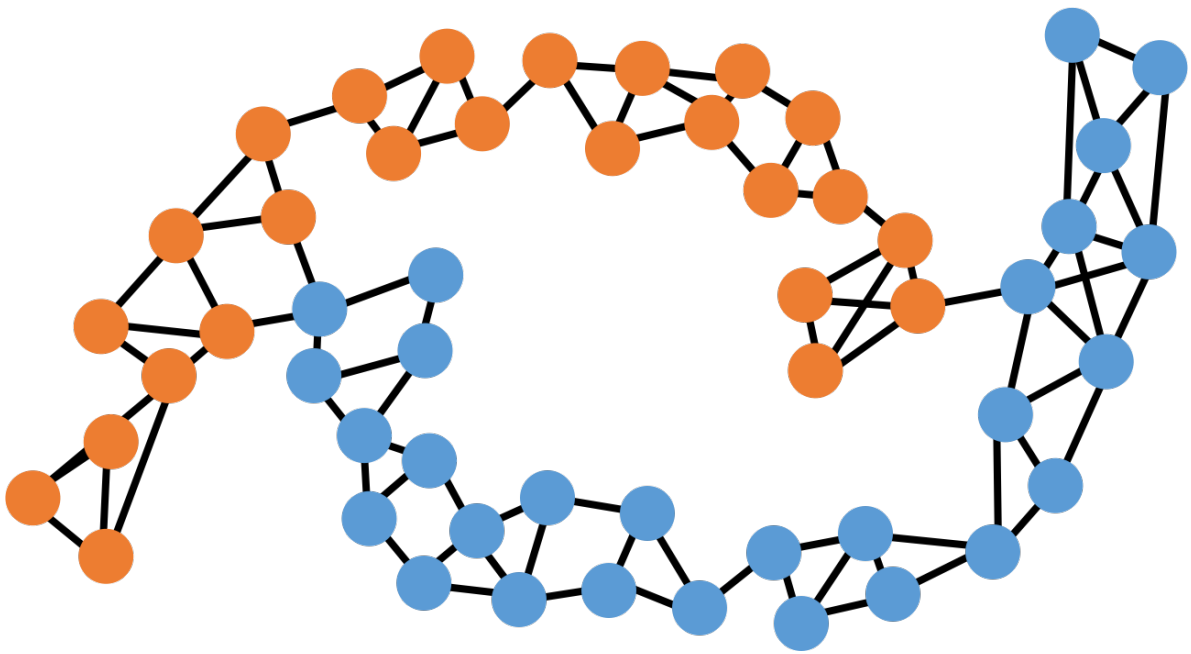

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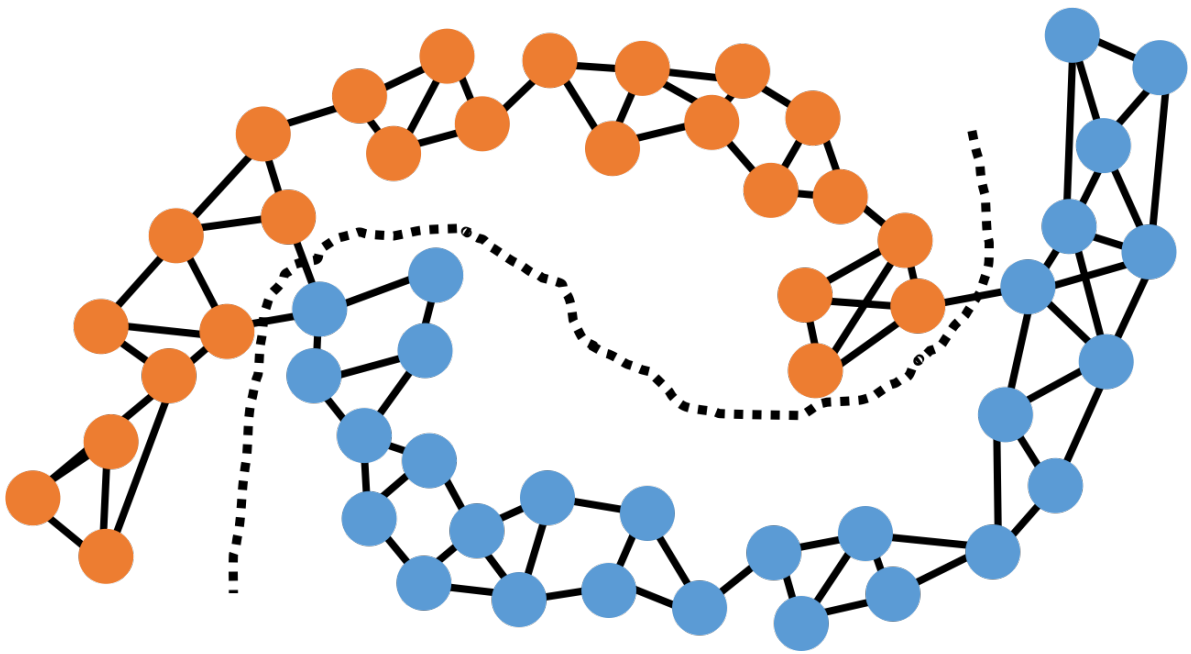

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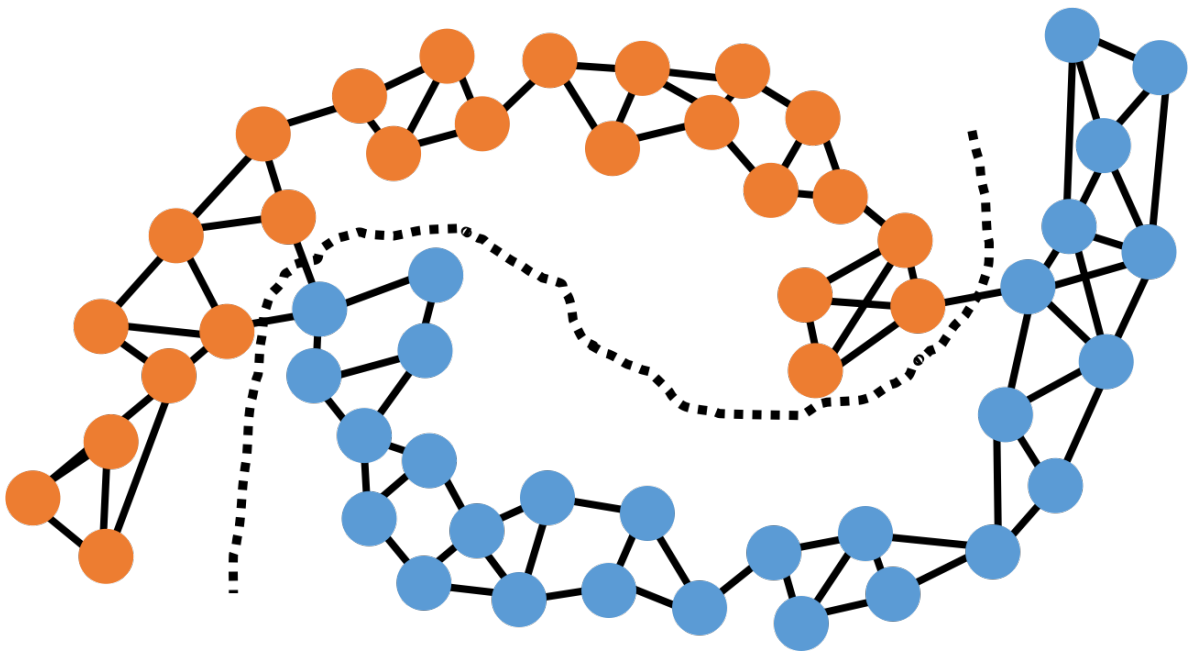
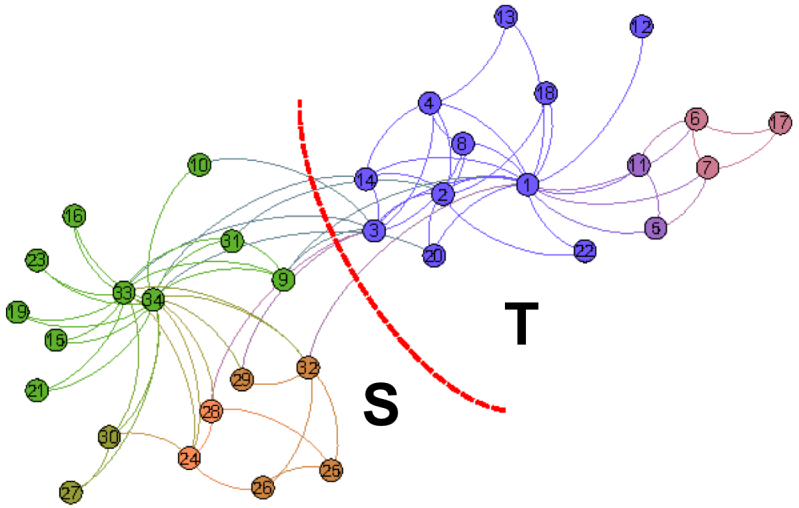


Can find this cut using eigendecomposition!

CUT MINIMIZATION

Simple Idea: Partition clusters along minimum cut in graph.



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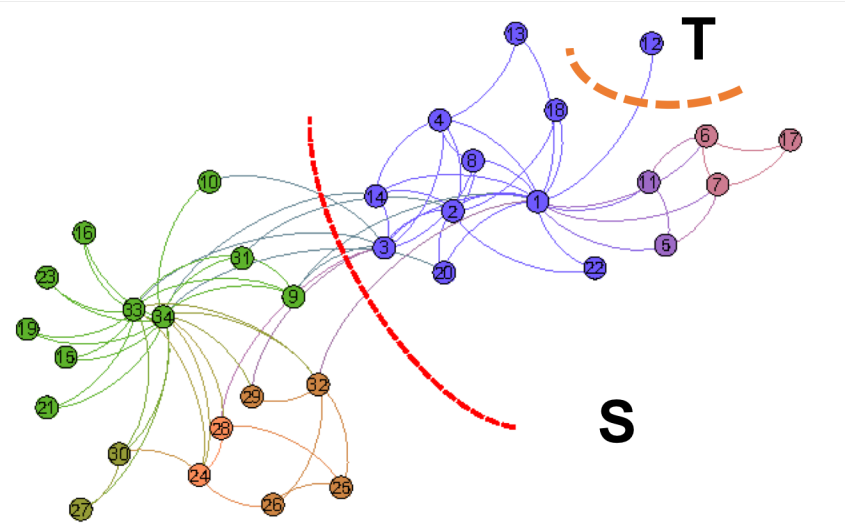

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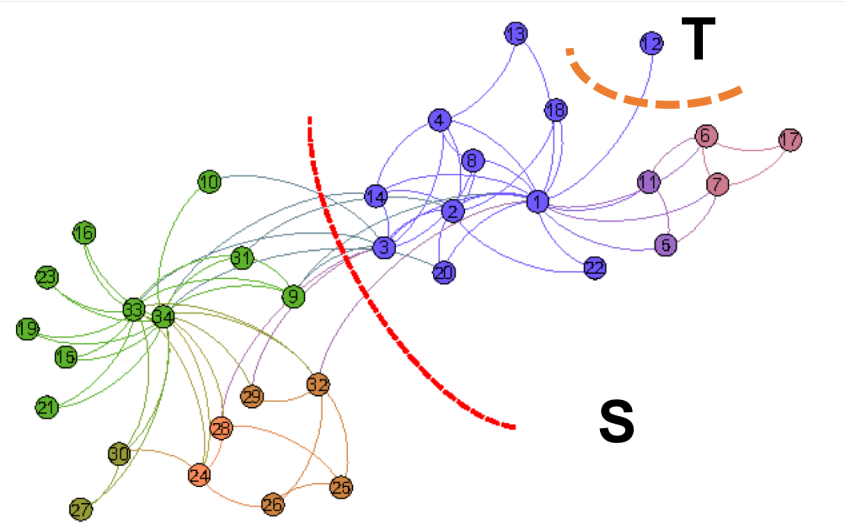

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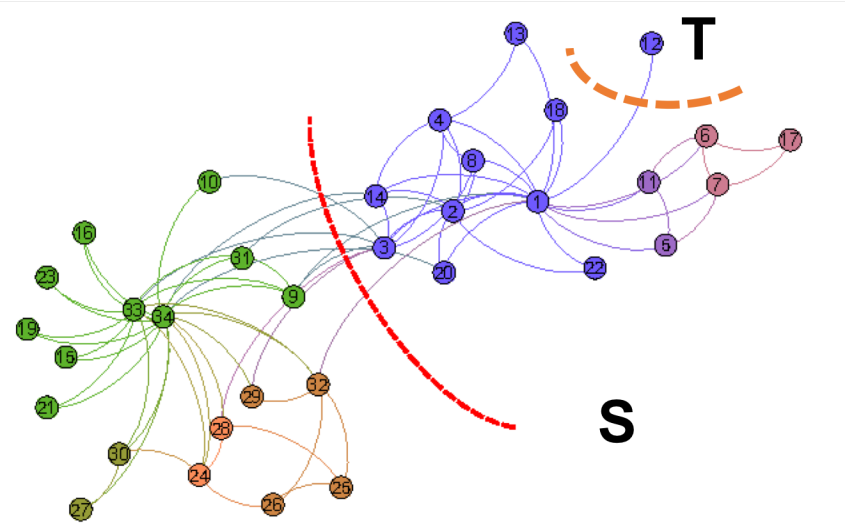

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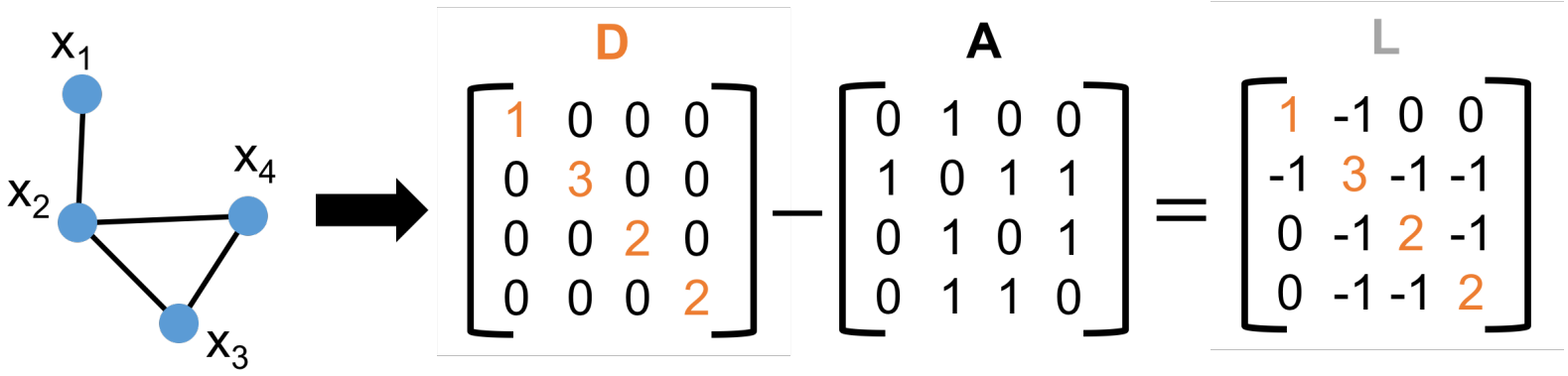
Small cuts are often not informative.

Solution: Encourage cuts that separate large sections of the graph.

- Let $\vec{v} \in \mathbb{R}^n$ be a cut indicator: $\vec{v}(i) = 1$ if $i \in S$. $\vec{v}(i) = -1$ if $i \in T$. Want $\vec{v}$ to have roughly equal numbers of 1s and -1s. I.e., $\vec{v}^T \vec{1} \approx 0$.

THE LAPLACIAN VIEW

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



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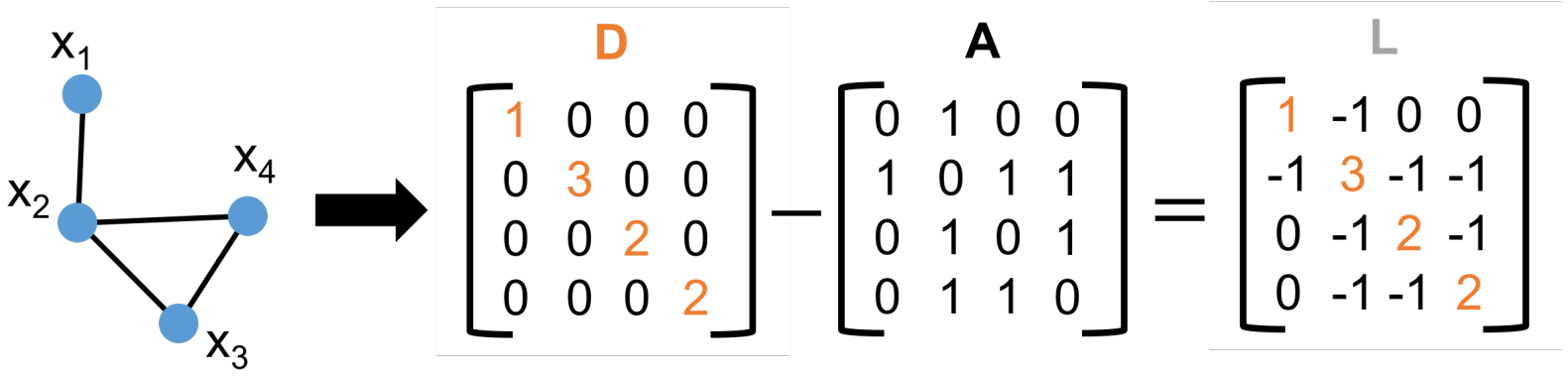

For any vector $\vec{v}$, its 'smoothness' over the graph is given by:

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

THE LAPLACIAN VIEW

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

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

SMALLEST LAPLACIAN EIGENVECTOR

Assuming the graph is connected, 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 eigenvalue $\vec{v}_n^T L \vec{v}_n = 0$.

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 $\mathbf{L} = \mathbf{D} - \mathbf{A}$.

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

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

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

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

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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.

CUTTING WITH THE SECOND LAPLACIAN EIGENVECTOR

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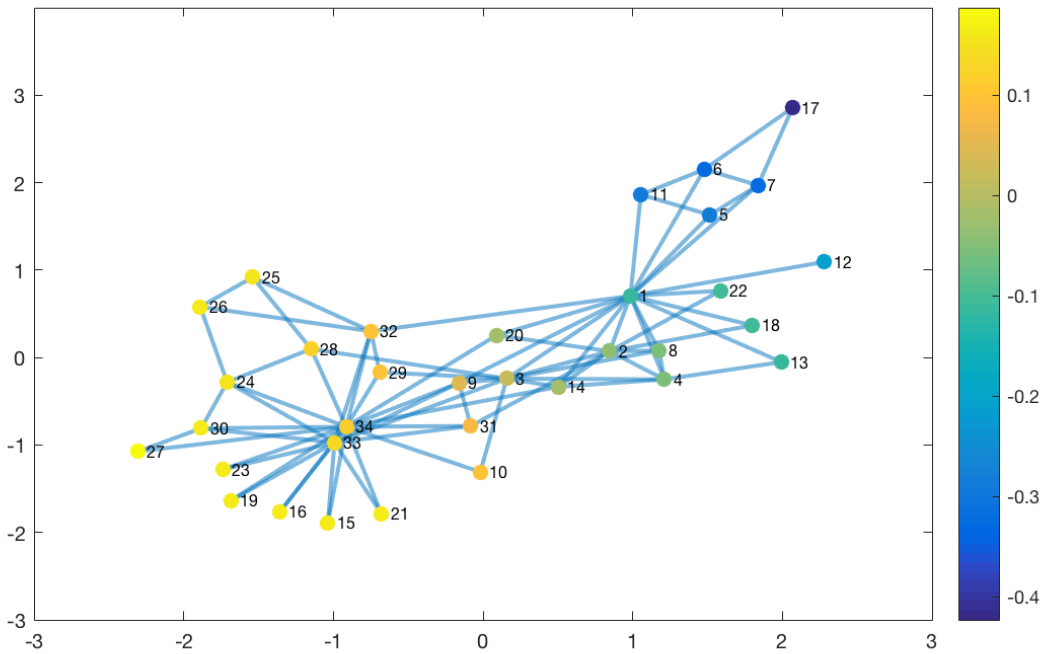

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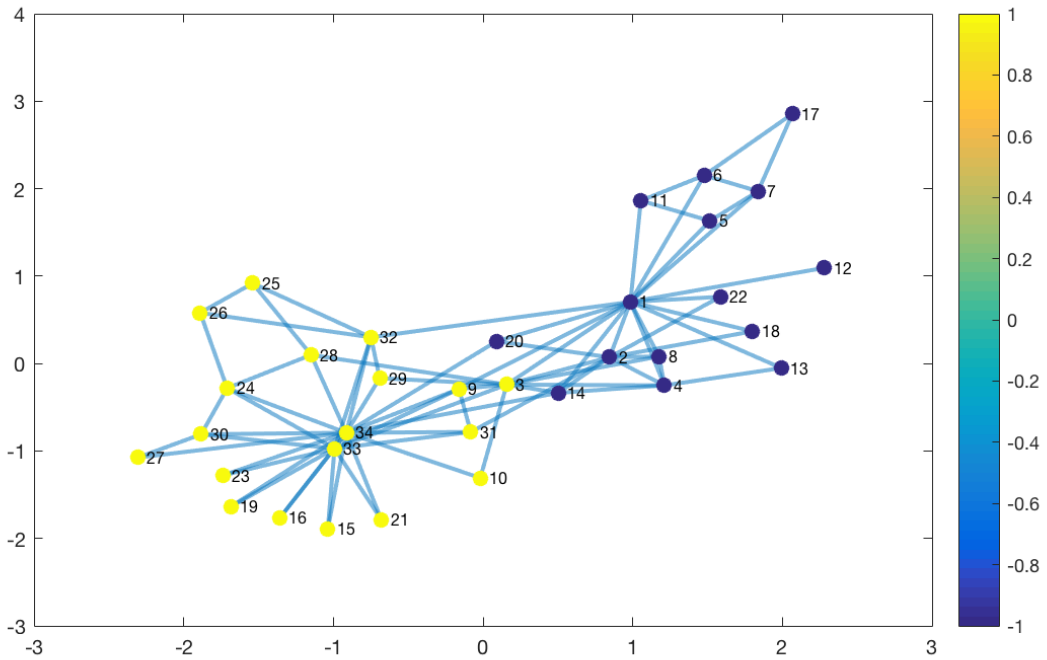

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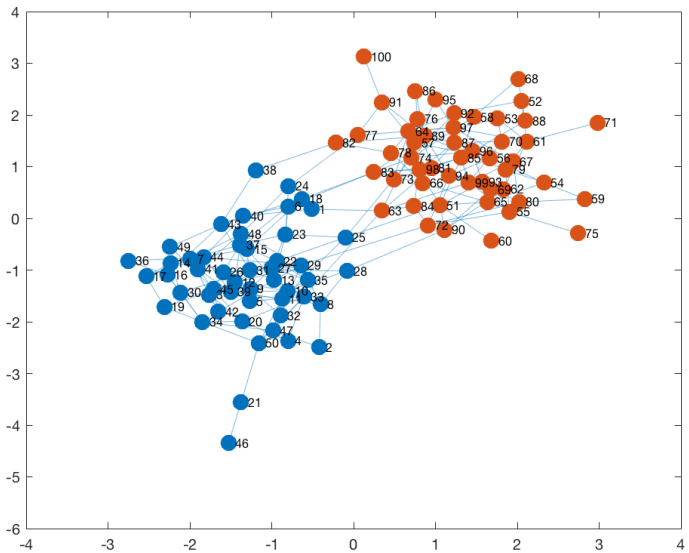
- Haven't given formal guarantees; it's difficult for general input graphs. But can consider randoms "natural" graphs...
- **Common Approach:** Give a natural generative model for random inputs and analyze how the algorithm performs on inputs drawn from this model. Can be used to justify ℓ_2 linear regression, k-means clustering, etc.

STOCHASTIC BLOCK MODEL

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.

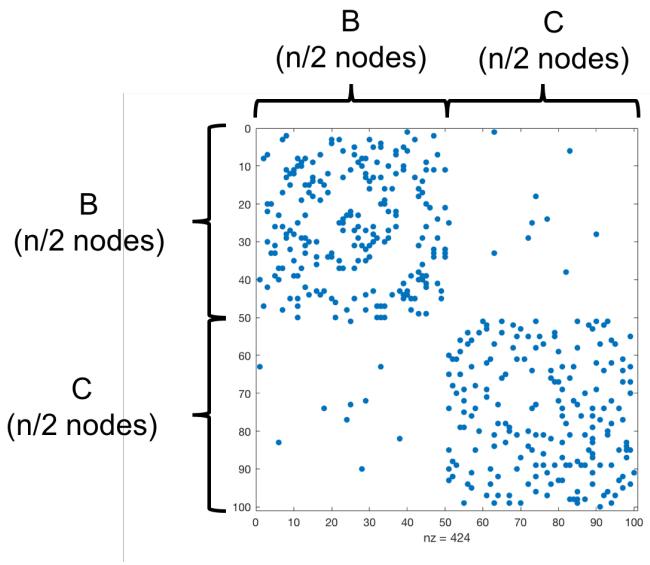
- Any two nodes in the same group are connected with probability p (including self-loops).
- Any two nodes in different groups are connected with prob. $q < p$.
- Connections are independent.

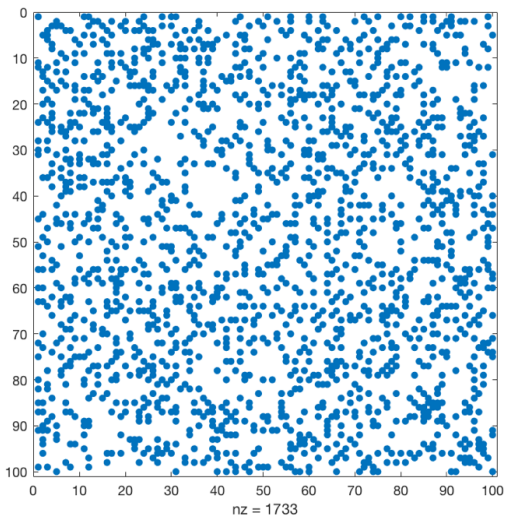


LINEAR ALGEBRAIC VIEW

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.

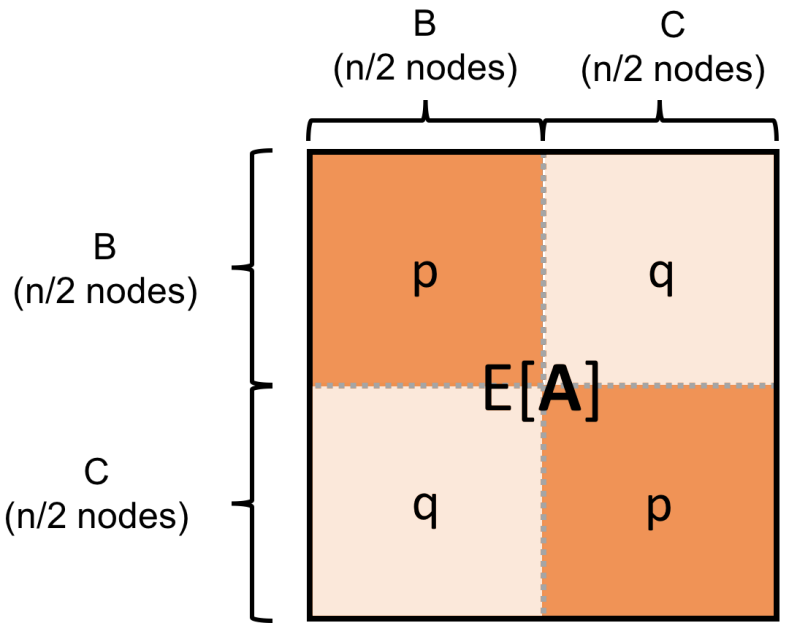




$G_n(p, q)$: stochastic block model distribution. B, C: groups with $n/2$ nodes each. Connections are independent with probability p between nodes in the same group, and probability q between nodes not in the same group.

EXPECTED ADJACENCY SPECTRUM

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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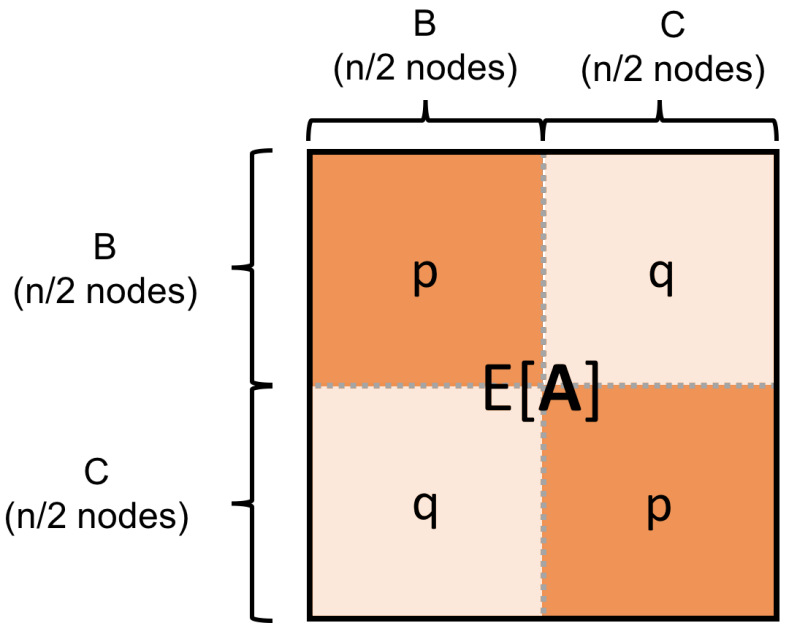

What is rank($\mathbb{E}[\mathbf{A}]$)? What are the eigenvectors and eigenvalues of $\mathbb{E}[\mathbf{A}]$?

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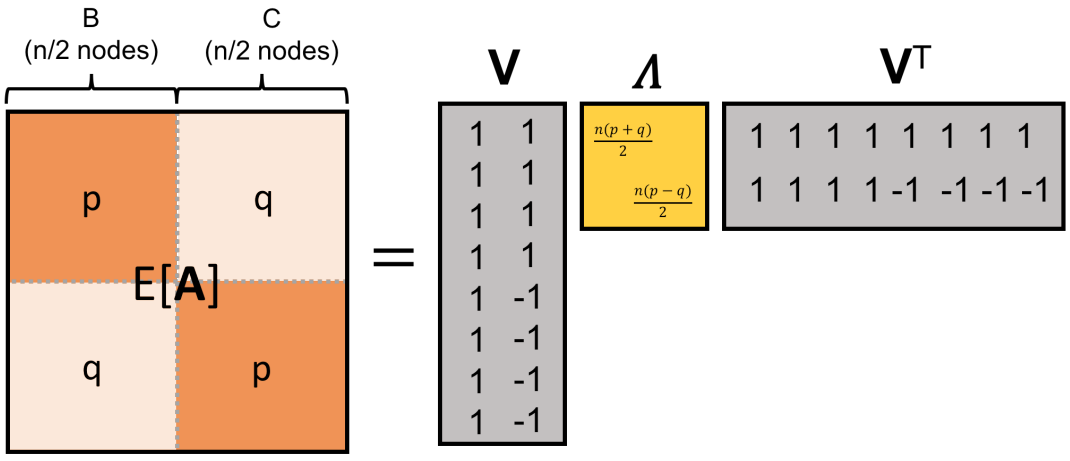

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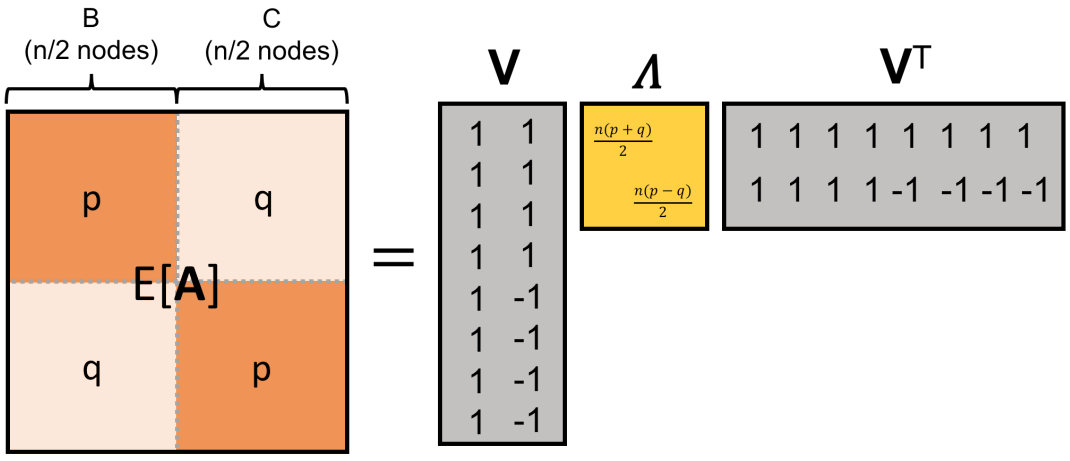

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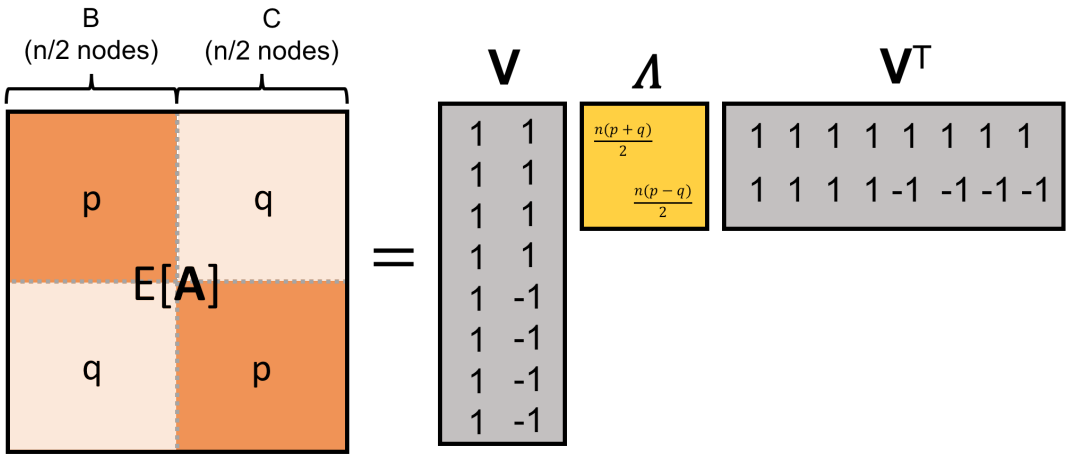

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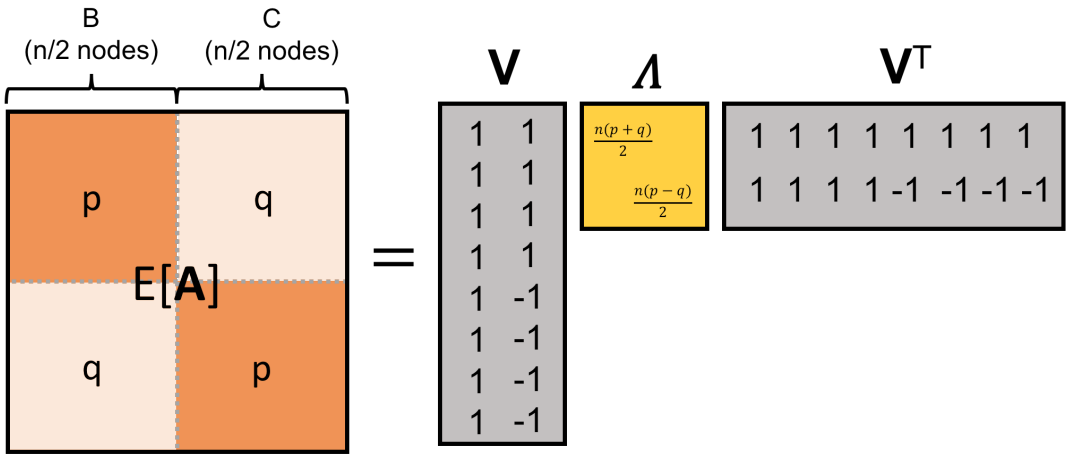

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- Second eigenvector of A is close to $[1, 1, 1, \ldots, -1, -1, -1]$ and gives a good estimate of the communities.

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

EXPECTED LAPLACIAN SPECTRUM

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 $\mathbb{E}[\mathbf{L}]$?

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Therefore the first and second eigenvalues of $\mathbb{E}[\mathbf{A}]$ are the second and first eigenvectors of $\mathbb{E}[\mathbf{L}]$.

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How do we show that a matrix is close to its expectation? Matrix concentration inequalities.

- Analogous to scalar concentration inequalities like Markovs, Chebyshevs, Bernsteins.
- Random matrix theory is a very recent and cutting edge subfield of mathematics that is being actively applied in computer science, statistics, and ML.

MATRIX CONCENTRATION

Matrix Concentration Inequality: If $p \geq O\left(\frac{\log^4 n}{n}\right)$, then with high probability

$$\|\mathbf{A} - \mathbb{E}[\mathbf{A}]\|_2 \leq O(\sqrt{pn}).$$

where $\|\cdot\|_2$ is the matrix spectral norm (operator norm).

For any $\mathbf{X} \in \mathbb{R}^{n \times d}$, $\|\mathbf{X}\|_2 = \max_{z \in \mathbb{R}^d : \|z\|_2 = 1} \|\mathbf{X}z\|_2$.

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For the stochastic block model application, we want to show that the second eigenvectors of $\mathbf{A}$ and $\mathbb{E}[\mathbf{A}]$ are close. How does this relate to their difference in spectral norm?

EIGENVECTOR PERTURBATION

Davis-Kahan Eigenvector Perturbation Theorem: Suppose $\mathbf{A}, \overline{\mathbf{A}} \in \mathbb{R}^{d \times d}$ are symmetric with $\|\mathbf{A} - \overline{\mathbf{A}}\|_2 \leq \epsilon$ and eigenvectors $v_1, v_2, \ldots, v_d$ and $\bar{v}_1, \bar{v}_2, \ldots, \bar{v}_d$. Letting $\theta(v_i, \bar{v}_i)$ denote the angle between v_i and $\bar{v}_i$, for all i:

$$\sin[\theta(v_i, \bar{v}_i)] \leq \frac{\epsilon}{\min_{j \neq i} |\lambda_i - \lambda_j|}$$

where $\lambda_1, \ldots, \lambda_d$ are the eigenvalues of $\overline{\mathbf{A}}$.

The errors get large if there's eigenvalues with similar magnitudes.

APPLICATION TO STOCHASTIC BLOCK MODEL

Claim 1 (Matrix Concentration): For $p \geq O\left(\frac{\log^4 n}{n}\right)$,

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Claim 2 (Davis-Kahan): For $p \geq O\left(\frac{\log^4 n}{n}\right)$,

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$\mathbf{A}$ adjacency matrix of random stochastic block model graph. p: connection probability within clusters. $q < p$: connection probability between clusters. n: number of nodes. $v_2, \bar{v}_2$: second eigenvectors of $\mathbf{A}$ and $\mathbb{E}[\mathbf{A}]$ respectively.

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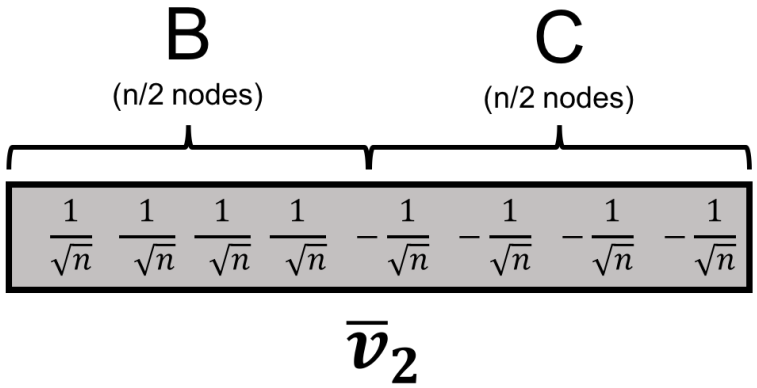

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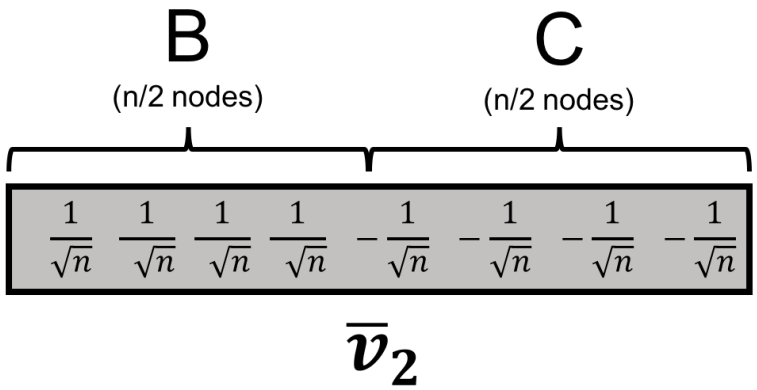

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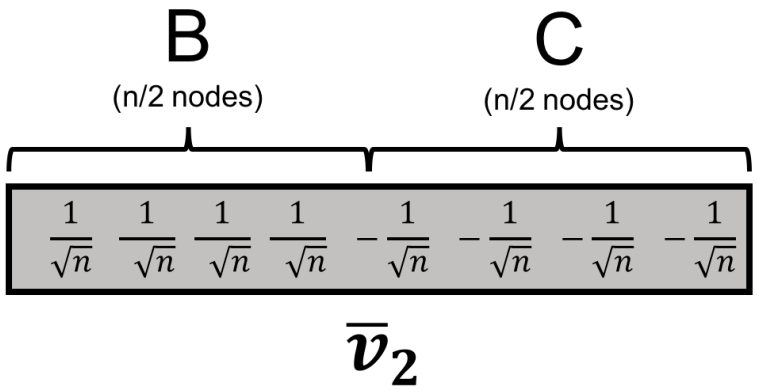

- Every i where $v_2(i)$, $\bar{v}_2(i)$ differ in sign contributes $\geq \frac{1}{n}$ to $\|v_2 - \bar{v}_2\|_2^2$.
- So they differ in sign in at most $O\left(\frac{p}{(p-q)^2}\right)$ positions.

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APPLICATION TO STOCHASTIC BLOCK MODEL

Upshot: If G is a stochastic block model graph with adjacency matrix **A**, if we compute its second large eigenvector v_2 and assign nodes to communities according to the sign pattern of this vector, we will correctly assign all but $O\left(\frac{p}{(p-q)^2}\right)$ nodes.