COMPSCI 514: ALGORITHMS FOR DATA SCIENCE

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University of Massachusetts Amherst. Fall 2019.

Lecture 16

Last Class:

- Spectral clustering and embeddings
- Started application to stochastic block model.

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This Class:

- Finish up stochastic block model.
- Efficient algorithms for SVD/eigendecomposition.
- Iterative methods: power method, Krylov subspace methods.

Goal: Argue the effectiveness of spectral clustering in a natural, if oversimplified, generative model.

STOCHASTIC BLOCK MODEL

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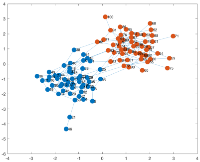
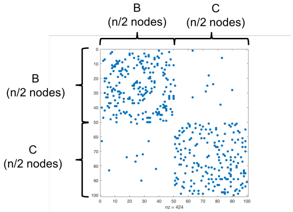
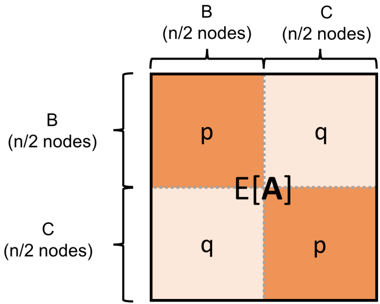
Stochastic Block Model (Planted Partition Model): Let $G_n(p, q)$ be a distribution over graphs on n nodes, split equally into two groups B and C, each with $n/2$ nodes.

- 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.





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.



$G_n(p,q)$: 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

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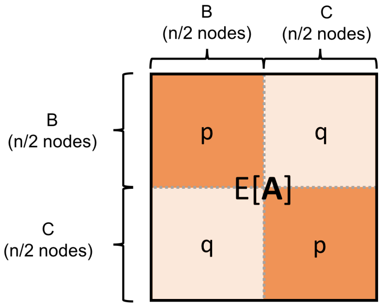

What is the rank of $\mathbb{E}[\mathbf{A}]$ and how can you see this quickly?

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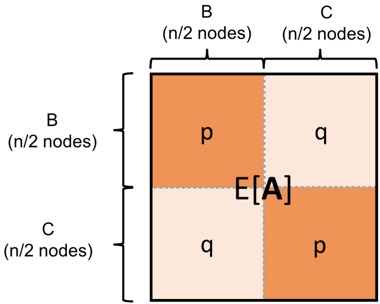

What is the rank of $\mathbb{E}[\mathbf{A}]$ and how can you see this quickly?
How many nonzero eigenvalues does $\mathbb{E}[\mathbf{A}]$ have?

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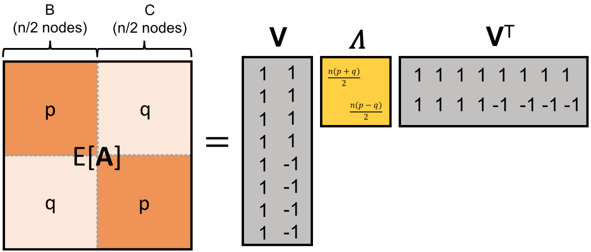

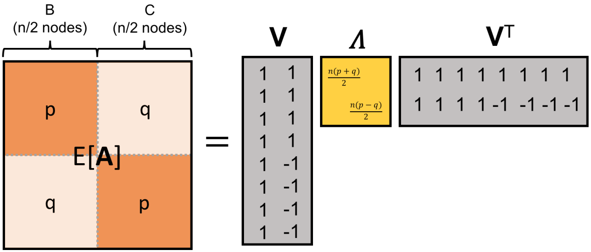

- $\vec{v}_1 = \vec{1}$ with eigenvalue $\lambda_1 = \frac{(p+q)n}{2}$.
- $\vec{v}_2 = \chi_{B,C}$ with eigenvalue $\lambda_2 = \frac{(p-q)n}{2}$.
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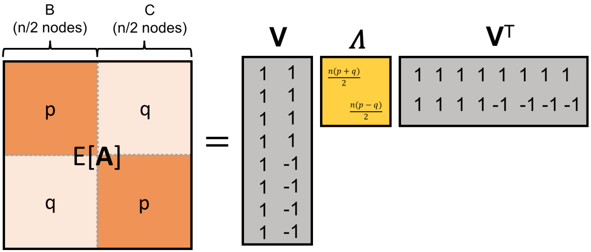

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If we compute $\vec{v}_2$ then we recover the communities B and C!

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

$$\mathbb{E}[L] = \mathbb{E}[D - A] = \mathbb{E}D - \mathbb{E}A$$

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

$$\mathbb{E}[L] = \underbrace{\frac{(p+q)n}{2} \cdot I}_{n \times n} - \underbrace{\left[\begin{array}{c|c} p & q \\ \hline q & p \end{array}\right]}_{n} \Big\} n$$

$$\mathbb{E}[L] = \left(\frac{(p+q)n}{2} I - \mathbb{E}[A]\right) v$$

$$= \underline{\frac{(p+q)n}{2}} v - \mathbb{E}[A] v \longrightarrow \mathbb{E}[L] v_i = \frac{(p+q)n}{2} v_i - \lambda_i v_i$$

v_i is eigenvector of $\mathbb{E}[A]$

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

$$\lambda_1 = \frac{(p+q)n}{2} \qquad \lambda_2 = \frac{(p-q)n}{2} \qquad \lambda_3, \lambda_4, \ldots = 0$$

$$\lambda_n(\mathbb{E}L) = 0 \qquad \lambda_{n-1}(\mathbb{E}L) = qn \qquad \lambda_{n-i}(\mathbb{E}L) \; \frac{(p+q)n}{2}$$

$$\text{rank}(\mathbb{E}L) = n-1$$

$$\text{rank}(\mathbb{E}[A]) = 2$$

$$\chi_{B,C} = [1 \; 1 \; 1 \; -1 \; -1 \; -1]$$

Upshot: The second small eigenvector of $\mathbb{E}[\mathbf{L}]$ is $\chi_{B,C}$ – the indicator vector for the cut between the communities.

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- Analogous to scalar concentration inequalities like Markovs, Chebyshevs, Bernsteins.

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How do we show that a matrix (e.g., $\mathbf{A}$) 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 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 $\mathbf{X} \in \mathbb{R}^{n \times d}$, $\|\mathbf{X}\|_2 = \max_{z \in \mathbb{R}^d : \|z\|_2 = 1} \|\mathbf{X}z\|_2$. ~ $z^T X^T X z$

top eigenvalue of $X^T X$

MATRIX CONCENTRATION

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Exercise: Show that $\|\mathbf{X}\|_2$ is equal to the largest singular value of $\mathbf{X}$. For symmetric $\mathbf{X}$ (like $\mathbf{A} - \mathbb{E}[\mathbf{A}]$) show that it is equal to the magnitude of the largest magnitude eigenvalue.

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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?

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:

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

$1,\ 1+\varepsilon$

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

The errors get large if there are eigenvalues with similar magnitudes.

$A = V \Lambda V^T$

$A = I A I^T$

$\|A - \bar{A}\|_2 = \varepsilon$

$$\underbrace{\begin{bmatrix} 1+\varepsilon & 0 \\ 0 & 1 \end{bmatrix}}_{\mathbf{A}} - \underbrace{\begin{bmatrix} 1 & 0 \\ 0 & 1+\varepsilon \end{bmatrix}}_{\bar{\mathbf{A}}} = \underbrace{\begin{bmatrix} \varepsilon & 0 \\ 0 & -\varepsilon \end{bmatrix}}_{\mathbf{A}-\bar{\mathbf{A}}}$$

$\left\| \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \right\| \to \left\| \begin{bmatrix} \varepsilon x_1 \\ -\varepsilon x_2 \end{bmatrix} \right\|$

$\lambda_1(A) = 1+\varepsilon$ $\qquad$ $\lambda_1(\bar{A}) = 1+\varepsilon$

$\lambda_2(A) = 1$ $\qquad$ $\lambda_2(\bar{A}) = 1$

$v_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, v_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$ $\qquad$ $\bar{v}_1 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \bar{v}_2 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$

$\sin\theta(v_1, \bar{v}_1) = 1 = \frac{\varepsilon}{\varepsilon}$ ⟵ $|\lambda_1 - \lambda_2|$

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

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

$$\sin\theta(v_2, \bar{v}_2) \leq \frac{O(\sqrt{pn})}{\min_{j \neq i} |\lambda_i - \lambda_j|}$$

$\mathbf{A}$ 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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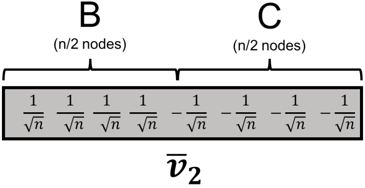

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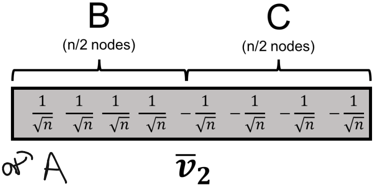

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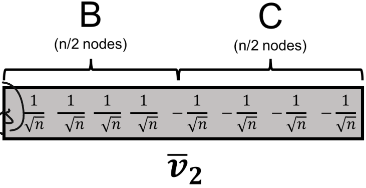

- Every i where $v_2(i), \bar{v}_2(i)$ differ in sign contributes $\geq \frac{1}{n}$ to $\|v_2 - \bar{v}_2\|_2^2$.
- So they differ in sign in at most $O\left(\frac{p}{(p-q)^2}\right)$ positions.

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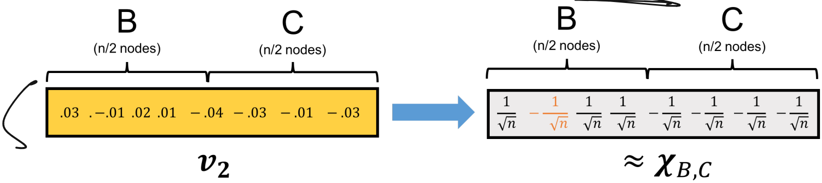
Upshot: If G is a stochastic block model graph with adjacency matrix $\mathbf{A}$, if we compute its second large eigenvector v_2 and assign nodes to communities according to the sign pattern of this vector, we will correctly assign all but $O\left(\frac{p}{(p-q)^2}\right)$ nodes.



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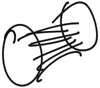

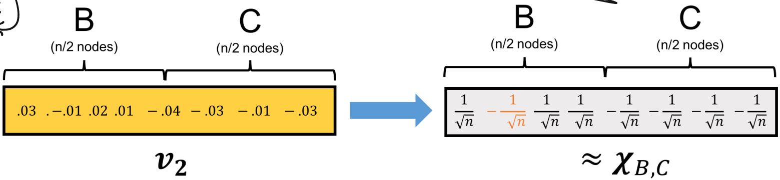

- Why does the error increase as q gets close to p?

$A = \begin{bmatrix} p & q \\ q & p \end{bmatrix}$ Generative models

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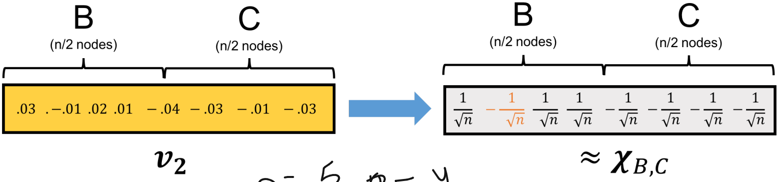

$p = .5$ $q = .4$ $O\left(\frac{p}{(p-q)^2}\right) = O(1)$

- Why does the error increase as q gets close to p?
- Even when $p - q = O(1/\sqrt{n})$, assign all but an $O(n)$ fraction of nodes correctly. E.g., assign 99% of nodes correctly.

$\frac{p}{(p-q)^2} = O(p \cdot n)$

Questions on spectral partitioning?

We have talked about the eigendecomposition and SVD as ways to compress data, to embed entities like words and documents, to compress/cluster non-linearly separable data.

How efficient are these techniques? Can they be run on massive datasets?

To compute the SVD of $\mathbf{A} \in \mathbb{R}^{n \times d}$, $\mathbf{A} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T$, first compute $\mathbf{V}$. Then compute $\mathbf{U}\boldsymbol{\Sigma} = \mathbf{A}\mathbf{V}$.

orthogonal columns diag

$$AV = U\Sigma V^T V = U\Sigma$$

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- Compute $\mathbf{A}^T\mathbf{A}$ – $O(nd^2)$ runtime. $d \times n \quad n \times d \to d \times d$

COMPUTING THE SVD

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UΣ

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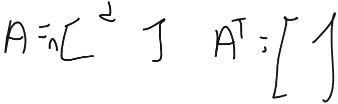

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- The worlds fastest super computers compute at ≈ 100 petaFLOPS = 10^{17} FLOPS (floating point operations per second).
- This is an easy task for them – but no one else.

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Won't cover: randomized methods, which can be much faster in some cases.

SPARSE VS. DIRECT

In numerical linear algebra, two main types of methods:

Direct Methods: Gaussian elimination, QR decomposition, Cholesky decomposition, etc.

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- Not just for sparse matrices!

SPARSE VS. DIRECT

Matlab:

`svd` and `eig` vs. `svds` and `eigs`

SciPy (Python):

`scipy.linalg.svd` vs. `scipy.sparse.linalg.svds`

direct (slow) — iterative (fast)

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- Choose $\vec{z}^{(0)}$ randomly. E.g. $\vec{z}^{(0)}(i) \sim \mathcal{N}(0, 1)$.
- For $i = 1, \ldots, t$
  - $\vec{z}^{(i)} = \mathbf{A}^T \cdot (\mathbf{A}\vec{z}^{(i-1)})$
  - $n_i = \|\vec{z}^{(i)}\|_2$
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Total Runtime: $O(ndt)$

Write $\vec{z}^{(0)}$ in the right singular vector basis:

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Claim:

$$\vec{z}^{(1)} = \frac{1}{n_1}\left[c_1 \cdot \sigma_1^2\vec{v}_1 + \mathbf{c}_2 \cdot \sigma_2^2\vec{v}_2 + \ldots + c_d \cdot \sigma_d^2\vec{v}_d\right]$$

Claim:

$$\vec{z}^{(t)} = \frac{1}{\prod_{i=1}^{t} n_i} \left[c_1 \cdot \sigma_1^{2t} \vec{v}_1 + \mathbf{c}_2 \cdot \sigma_2^{2t} \vec{v}_2 + \ldots + c_d \cdot \sigma_d^{2t} \vec{v}_d \right]$$

After t iterations, you have 'powered' up the singular values, making the component in the direction of v_1 much larger, relative to the other components.

Theorem (Basic Power Method Convergence)

Let $\gamma = \frac{\sigma_1 - \sigma_2}{\sigma_1}$ *be parameter capturing the "gap" between the first and second largest singular values. If Power Method is initialized with a random Gaussian vector then, with high probability, after* $t = O\left(\frac{\log d/\epsilon}{\gamma}\right)$ *steps:*

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Next Time: Will analyze this method formally.