CS-GY 9223 I: Lecture 10
Krylov methods, spectral clustering, spectral graph theory.

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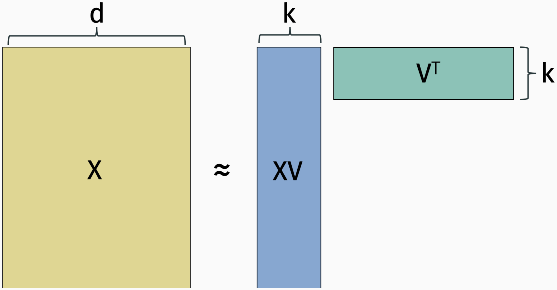
COMPUTATION IN LINEAR ALGEBRA

Three classes of methods.

- Direct Methods:
- Iterative Methods:
- Randomized Methods:

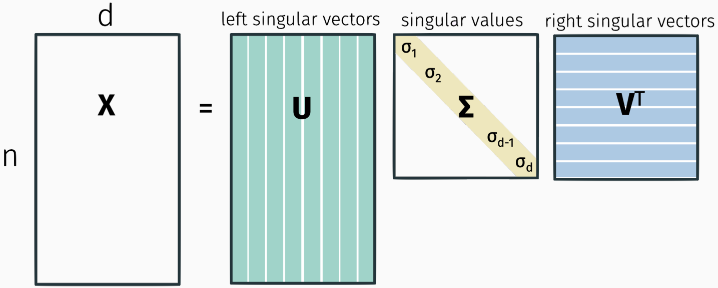
LOW-RANK APPROXIMATION

Write $\mathbf{X}$ as a rank k factorization by projecting onto the subspace spanned by an orthanormal matrix $\mathbf{V} \in \mathbb{R}^{d \times k}$



One-stop shop for computing optimal low-rank approximations.

Any matrix **X** can be written:



Where $\mathbf{U}^T\mathbf{U} = \mathbf{I}$, $\mathbf{V}^T\mathbf{V} = \mathbf{I}$, and $\sigma_1 \geq \sigma_2 \geq \ldots \sigma_d \geq 0$.

COMPUTATIONAL QUESTION

Given a subspace $\mathcal{V}$ spanned by the k columns in $\mathbf{V}$,

$$\|\mathbf{X}-\mathbf{X}\mathbf{V}\mathbf{V}^T\|_F^2 = \min_{\mathbf{C}} \|\mathbf{X}-\mathbf{C}\mathbf{V}^T\|_F^2$$

We want to find the best $\mathbf{V} \in \mathbb{R}^{d\times k}$:

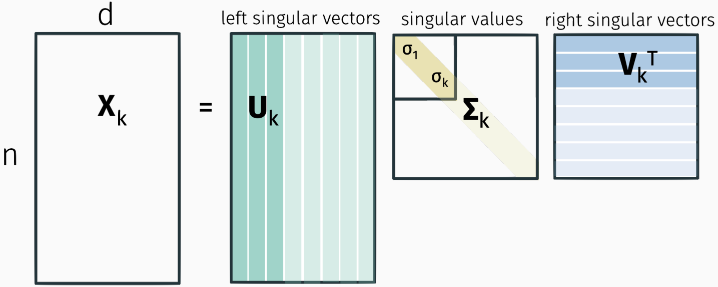
$$\min_{\text{orthonormal } \mathbf{V}\in\mathbb{R}^{d\times k}} \|\mathbf{X}-\mathbf{X}\mathbf{V}\mathbf{V}^T\|_F^2 \tag{1}$$

Note that $\|\mathbf{X}-\mathbf{X}\mathbf{V}\mathbf{V}^T\|_F^2 = \|\mathbf{X}\|_F^2 - \|\mathbf{X}\mathbf{V}\mathbf{V}^T\|_F^2$ for all orthonormal $\mathbf{V}$ (since $\mathbf{V}\mathbf{V}^T$ is a projection). Equivalent form:

$$\max_{\text{orthonormal } \mathbf{V}\in\mathbb{R}^{d\times k}} \|\mathbf{X}\mathbf{V}\mathbf{V}^T\|_F^2 = \|\mathbf{X}\mathbf{V}\|_F^2 \tag{2}$$

SINGULAR VALUE DECOMPOSITION

Can read off optimal low-rank approximations from the SVD:



$$\mathbf{X}_k = \mathbf{U}_k \mathbf{U}_k^T \mathbf{X} = \mathbf{X}\mathbf{V}_k\mathbf{V}_k^T.$$

$$\mathbf{V}_k = \underset{\text{orthonormal } \mathbf{V} \in \mathbb{R}^{d \times k}}{\arg\min} \|\mathbf{X} - \mathbf{X}\mathbf{V}\mathbf{V}^T\|_F^2 = \underset{\text{orthonormal } \mathbf{V} \in \mathbb{R}^{d \times k}}{\arg\max} \|\mathbf{X}\mathbf{V}\mathbf{V}^T\|_F^2$$

POWER METHOD

Goal: Find some $\mathbf{z} \approx \mathbf{v}_1$.

Input: $\mathbf{X} \in \mathbb{R}^{n \times d}$ with SVD $\mathbf{U\Sigma V}$.

Power method:

- Choose $\mathbf{z}^{(0)}$ randomly. E.g. $\mathbf{z}_0 \sim \mathcal{N}(0, 1)$.
- For $i = 1, \ldots, T$
    - $\mathbf{z}^{(i)} = \mathbf{X}^T \cdot (\mathbf{X}\mathbf{z}^{(i-1)})$
    - $n_i = \|\mathbf{z}^{(i)}\|_2$
    - $\mathbf{z}^{(i)} = \mathbf{z}^{(i)} / n_i$

  Return $\mathbf{z}_T$

POWER METHOD CONVERGENCE

Theorem (Power Method Convergence)

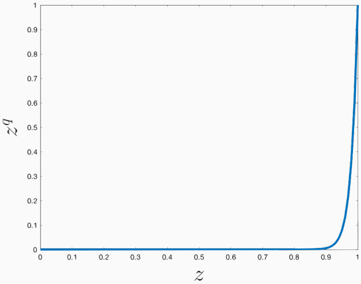
Let $\gamma = \frac{\sigma_1 - \sigma_2}{\sigma_1}$ be parameter capturing the "gap" between the first and second largest singular values. If Power Method is initialized with a random Gaussian vector then, with high probability, after $T = O\left(\frac{\log d/\epsilon}{\gamma}\right)$ steps, we have:

$$\|\mathbf{v}_1 - \mathbf{z}^{(T)}\|_2 \leq \epsilon.$$

Total runtime: $O(T \cdot \text{nnz}(\mathbf{X})) \leq O(T \cdot nd)$

KRYLOV SUBSPACE METHODS

$$\mathbf{z}^{(q)} = c \cdot \left(\mathbf{X}^T\mathbf{X}\right)^q \cdot \mathbf{g}$$



$$\mathbf{z}^{(q)} = c \cdot \left[c_1 \cdot \sigma_1^{2q}\mathbf{v}_1 + c_2 \cdot \sigma_2^{2q}\mathbf{v}_2 + \ldots + c_n \cdot \sigma_n^{2q}\mathbf{v}_n\right]$$

KRYLOV SUBSPACE METHODS

$$\mathbf{z}^{(q)} = c \cdot \left(\mathbf{X}^T\mathbf{X}\right)^q \cdot \mathbf{g}$$

Along the way we computed:

$$\mathcal{K}_q = \left[\mathbf{g}, (\mathbf{X}^T\mathbf{X}) \cdot \mathbf{g}, \left(\mathbf{X}^T\mathbf{X}\right)^2 \cdot \mathbf{g}, \ldots, \left(\mathbf{X}^T\mathbf{X}\right)^q \cdot \mathbf{g}\right]$$

$\mathcal{K}$ is called the Krylov subspace of degree q.

Idea behind Krlyov methods: Don’t throw away everything before $\left(\mathbf{X}^T\mathbf{X}\right)^q \cdot \mathbf{g}$. What you’re using when you run `svds` or `eigs` in MATLAB or Python.

KRYLOV SUBSPACE METHODS

Want to find $\mathbf{v}$, which minimizes $\|\mathbf{X} - \mathbf{X}\mathbf{v}\mathbf{v}^T\|_F^2$.

Lanczos method:

- Let $\mathbf{Q} \in \mathbb{R}^{d \times k}$ be an orthonormal span for the vectors in $\mathcal{K}$.
- Solve $\min_{\mathbf{v}=\mathbf{Q}\mathbf{w}} \|\mathbf{X} - \mathbf{X}\mathbf{v}\mathbf{v}^T\|_F^2$.
    - Find <u>best</u> vector in the Krylov subspace, instead of just using last vector.
    - Can be done in $O\left(\mathrm{nnz}(\mathbf{X}) \cdot k + dk^2\right)$ time.

LANCZOS METHOD ANALYSIS

Claim 1: For any degree q polynomial p, we can write $p(\mathbf{X}^T\mathbf{X}) \cdot \mathbf{g}$ as $\mathbf{Q}\mathbf{w}$ for some $\mathbf{w}$.

Claim 2:

$$\min_{\mathbf{v}=\mathbf{Q}\mathbf{w}} \|\mathbf{X} - \mathbf{X}\mathbf{v}\mathbf{v}^T\|_F^2 = \min_{\text{degree } q \text{ polynomial} p} \|\mathbf{X} - \mathbf{X}\mathbf{v}_p\mathbf{v}_p^T\|_F^2$$

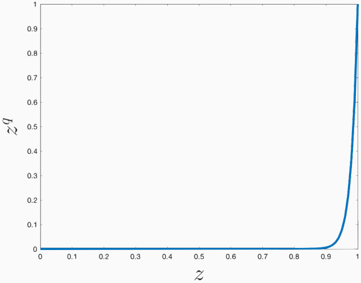
where $\mathbf{v}_p = p(\mathbf{X}^T\mathbf{X}) \cdot \mathbf{g}$.

Claim 3:

$$\mathbf{z}^{(q)} = c \cdot \left[c_1 \cdot p(\sigma_1^2)\mathbf{v}_1 + c_2 \cdot p(\sigma_2^2)\mathbf{v}_2 + \ldots + c_n \cdot p(\sigma_n^2)\mathbf{v}_n\right]$$

LANCZOS METHOD ANALYSIS

Claim: There is an $O\left(\sqrt{q \log \frac{1}{\epsilon}}\right)$ degree polynomial $\hat{p}$ approximating $\mathbf{x}^q$ up to error ϵ on $[0, \sigma_1^2]$.



$$\|\mathbf{X} - \mathbf{X}\mathbf{v}_{p*}\mathbf{v}_{p*}^T\|_F^2 \leq \|\mathbf{X} - \mathbf{X}\mathbf{v}_{\hat{p}}\mathbf{v}_{\hat{p}}^T\|_F^2 \approx \|\mathbf{X} - \mathbf{X}\mathbf{v}_{x^q}\mathbf{v}_{x^q}^T\|_F^2 \approx \|\mathbf{X} - \mathbf{X}\mathbf{v}_1\mathbf{v}_1^T\|_F^2$$

Runtime: $O\left(\frac{\log(d/\epsilon)}{\sqrt{\gamma}} \cdot \text{nnz}(\mathbf{X})\right)$ vs. $O\left(\frac{\log(d/\epsilon)}{\gamma} \cdot \text{nnz}(\mathbf{X})\right)$

POWER METHOD – NO GAP DEPENDENCE

Convergence is slow when $\gamma = \frac{\sigma_1-\sigma_2}{\sigma_1}$ is small. $\mathbf{z}^{(q)}$ has large components of both $\mathbf{v}_1$ and $\mathbf{v}_2$. But in this case:

$$\|\mathbf{X} - \mathbf{X}\mathbf{v}_1\mathbf{v}_1^T\|_F^2 = \sum_{i\neq 1}\sigma_i^2 \approx \sum_{i\neq 2} = \sigma_i^2 \|\mathbf{X} - \mathbf{X}\mathbf{v}_2\mathbf{v}_2^T\|_F^2.$$

So we don't care! Either $\mathbf{v}_1$ or $\mathbf{v}_2$ give good rank-1 approximations.

Claim: To achieve

$$\|\mathbf{X} - \mathbf{X}\mathbf{z}\mathbf{z}^T\|_F^2 \leq (1+\epsilon)\|\mathbf{X} - \mathbf{X}\mathbf{v}_1\mathbf{v}_1^T\|_F^2$$

we need $O\left(\frac{\log(d/\epsilon)}{\epsilon}\right)$ power method iterations or $O\left(\frac{\log(d/\epsilon)}{\sqrt{\epsilon}}\right)$ Lanczos iterations.

GENERALIZATIONS TO LARGER k

- Block Power Method aka Simultaneous Iteration aka Subspace Iteration aka Orthogonal Iteration
- Block Krylov methods

- Let $\mathbf{G} \in \mathbb{R}^{d \times k}$ be a random Gaussian matrix.
- $\mathcal{K}_q = \left[\mathbf{G}, (\mathbf{X}^T\mathbf{X}) \cdot \mathbf{G}, (\mathbf{X}^T\mathbf{X})^2 \cdot \mathbf{G}, \ldots, (\mathbf{X}^T\mathbf{X})^q \cdot \mathbf{G}\right]$

Runtime: $O\left(\text{nnz}(\mathbf{X}) \cdot k \cdot \frac{\log d/\epsilon}{\sqrt{\epsilon}}\right)$ to obtain a nearly optimal low-rank approximation.

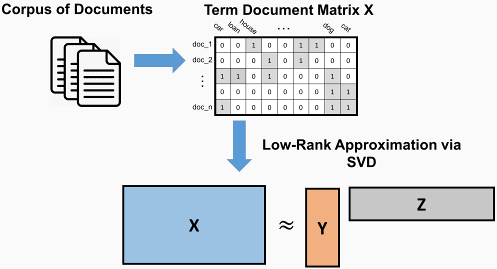
What do you think a stochastic version of Krylov subspace method would look like?

$$\mathcal{K}_q = \left[\mathbf{g}, (\mathbf{X}^T\mathbf{X}) \cdot \mathbf{g}, (\mathbf{X}^T\mathbf{X})^2 \cdot \mathbf{g}, \ldots, (\mathbf{X}^T\mathbf{X})^q \cdot \mathbf{g}\right]$$

Applications of (partial) singular value decomposition:

- Low-rank approximation (data compression)
- Denoising, in-painting, matrix completion
- Semantic embeddings

EXAMPLE: LATENT SEMANTIC ANALYSIS



Corpus of Documents

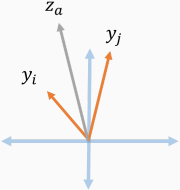
Term Document Matrix X

	car	loan	house		…			dog	cat
doc_1	0	0	1	0	0	1	1	0	0
doc_2	0	0	0	1	0	1	0	0	0
⋮	1	1	0	1	0	0	0	1	0
	0	0	0	0	0	0	0	1	1
doc_n	1	0	0	0	0	0	0	1	1

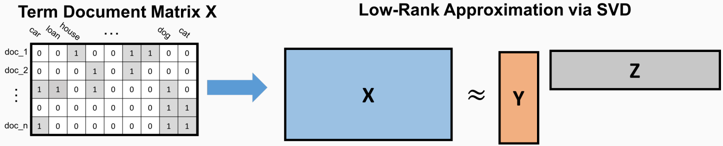
Low-Rank Approximation via SVD

X ≈ Y Z

- $\langle \vec{y}_i, \vec{z}_a \rangle \approx 1$ when doc_i contains $word_a$.
- If doc_i and doc_j both contain $word_a$, $\langle \vec{y}_i, \vec{z}_a \rangle \approx \langle \vec{y}_j, \vec{z}_a \rangle = 1$.



EXAMPLE: LATENT SEMANTIC ANALYSIS



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⋮	1	1	0	1	0	0	0	1	0
	0	0	0	0	0	0	0	1	1
doc_n	1	0	0	0	0	0	0	1	1

Low-Rank Approximation via SVD

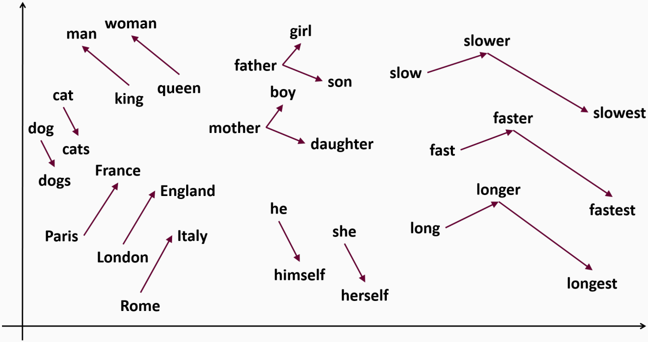
- The columns $\vec{z}_1, \vec{z}_2, \ldots$ give representations of words, with $\vec{z}_i$ and $\vec{z}_j$ tending to have high dot product if $word_i$ and $word_j$ appear in many of the same documents.
- $\mathbf{Z}$ corresponds to the top k right singular vectors: the eigenvectors of $\mathbf{X}\mathbf{X}^T$. Intuitively, what is $\mathbf{X}\mathbf{X}^T$?
- $(\mathbf{X}\mathbf{X}^T)_{i,j} =$

EXAMPLE: WORD EMBEDDING

Not obvious how to convert a word into a feature vector that captures the meaning of that word. Approach suggested by LSA: build a $d \times d$ symmetric “similarity matrix” $\mathbf{M}$ between words, and factorize: $\mathbf{M} \approx \mathbf{F}\mathbf{F}^T$ for rank k $\mathbf{F}$.

- **Similarity measures:** How often do $word_i, word_j$ appear in the same sentence, in the same window of w words, in similar positions of documents in different languages?
- Replacing $\mathbf{X}\mathbf{X}^T$ with these different metrics (sometimes appropriately transformed) leads to popular word embedding algorithms: `word2vec`, `GloVe`, etc.

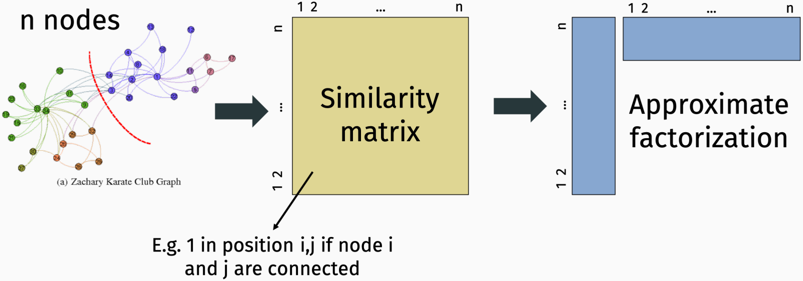
example: ord Embedding



`word2vec` was originally described as a neural-network method, but Levy and Goldberg show that it is simply low-rank approximation of a specific similarity matrix. *Neural word embedding as implicit matrix factorization.*

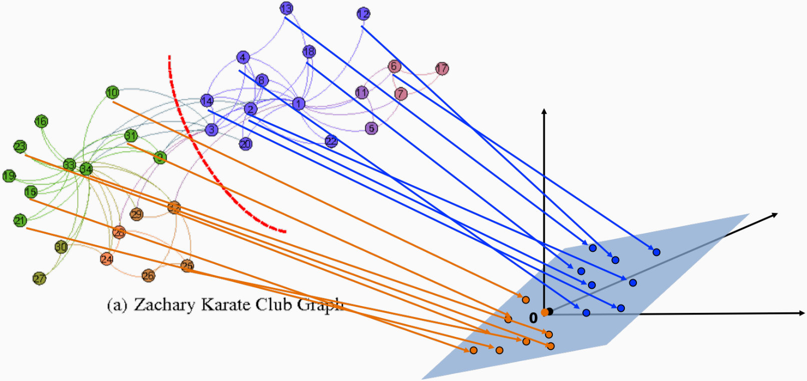
ENCODING GRAPH SIMILARITY

Often data is represented as a graph and similarities can be obtained from that graph:



n nodes
(a) Zachary Karate Club Graph
1 2 ... n
n ... 1 2
Similarity matrix
E.g. 1 in position i,j if node i and j are connected
Approximate factorization

ENCODING GRAPH SIMILARITY

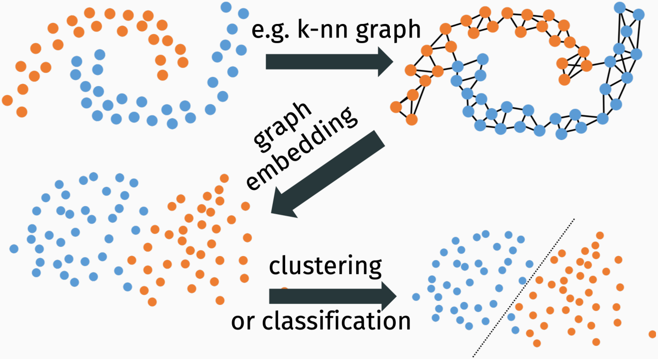


ZACHARY KARATE CLUB DRAMA

Social networks in 1970: “The network captures 34 members of a karate club, documenting links between pairs of members who interacted outside the club. During the study a conflict arose between the administrator ”John A” and instructor ”Mr. Hi” (pseudonyms), which led to the split of the club into two. Half of the members formed a new club around Mr. Hi; members from the other part found a new instructor or gave up karate. Based on collected data Zachary correctly assigned all but one member of the club to the groups they actually joined after the split.” – Wikipedia

SPECTRAL CLUSTERING

Idea: Construct synthetic graph for data that is hard to cluster.



Spectral Clustering, Laplacian Eigenmaps, Locally linear embedding, Isomap, etc.

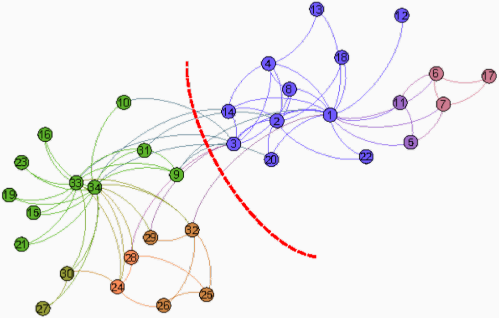
SPECTRAL GRAPH THEORY

Spectral graph theory lets us formalize this heuristic idea.

CUT MINIMIZATION

Goal: Partition nodes along a cut that:

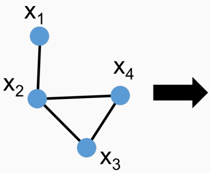
- Has few crossing edges: $|\{(u,v) \in E : u \in S, v \in T\}|$ is small.
- Separates large partitions: $|S|, |T|$ are not too small.



(a) Zachary Karate Club Graph

THE LAPLACIAN VIEW

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



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

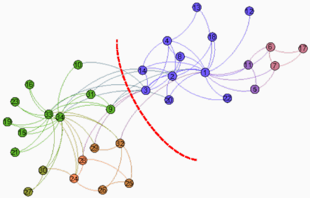
$\mathbf{L} = \mathbf{B}^T\mathbf{B}$ where B is the “edge-vertex incidence” matrix.

$\mathbf{B} =$

Conclusions from $\mathbf{L} = \mathbf{B}^T\mathbf{B}$

- $\mathbf{L}$ is positive semidefinite: $\mathbf{x}^T\mathbf{L}\mathbf{x} \geq 0$ <u>for all</u> $\mathbf{x}$.
- $\mathbf{L} = \mathbf{V}\mathbf{\Sigma}^2\mathbf{V}^T$ where $\mathbf{U}\mathbf{\Sigma}^2\mathbf{V}^T$ is $\mathbf{B}$'s SVD. Columns of $\mathbf{V}$ are <u>eigenvectors</u> of $\mathbf{L}$.
- For a <u>cut indicator vector</u> $\mathbf{c} \in \{-1, 1\}^n$ with $\mathbf{c}(i) = -1$ for $i \in S$ and $\mathbf{c}(i) = 1$ for $i \in T$:
  - $\mathbf{c}^T L\mathbf{c} = \sum_{(i,j)\in E}(\mathbf{c}(i) - \mathbf{c}(j))^2 = 4 \cdot cut(S, T)$.

THE LAPLACIAN VIEW



(a) Zachary Karate Club Graph

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

- $\mathbf{c}^T L \mathbf{c} = 4 \cdot cut(S, T)$.
- $\mathbf{c}^T \mathbf{1} = |T| - |S|$.

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

Courant–Fischer min-max principle

Let $\mathbf{V} = [\mathbf{v}_1, \ldots, \mathbf{v}_n]$ be the eigenvectors of $\mathbf{L}$.

$$
\begin{aligned}
\mathbf{v}_1 &= \arg\max_{\|\mathbf{v}\|=1} \mathbf{v}^T\mathbf{L}\mathbf{v} \\
\mathbf{v}_2 &= \arg\max_{\|\mathbf{v}\|=1, \mathbf{v}\perp\mathbf{v}_1} \mathbf{v}^T\mathbf{L}\mathbf{v} \\
\mathbf{v}_3 &= \arg\max_{\|\mathbf{v}\|=1, \mathbf{v}\perp\mathbf{v}_1, \mathbf{v}_2} \mathbf{v}^T\mathbf{L}\mathbf{v} \\
&\vdots \\
\mathbf{v}_n &= \arg\max_{\|\mathbf{v}\|=1, \mathbf{v}\perp\mathbf{v}_1, \ldots, \mathbf{v}_{n-1}} \mathbf{v}^T\mathbf{L}\mathbf{v}
\end{aligned}
$$

Courant–Fischer min-max principle

Let $\mathbf{V} = [\mathbf{v}_1, \ldots, \mathbf{v}_n]$ be the eigenvectors of $\mathbf{L}$.

$$
\begin{aligned}
\mathbf{v}_n &= \operatorname*{arg\,min}_{\|\mathbf{v}\|=1} \mathbf{v}^T \mathbf{L} \mathbf{v} \\
\mathbf{v}_{n-1} &= \operatorname*{arg\,min}_{\|\mathbf{v}\|=1, \mathbf{v} \perp \mathbf{v}_n} \mathbf{v}^T \mathbf{L} \mathbf{v} \\
\mathbf{v}_{n-2} &= \operatorname*{arg\,min}_{\|\mathbf{v}\|=1, \mathbf{v} \perp \mathbf{v}_n, \mathbf{v}_{n-1}} \mathbf{v}^T \mathbf{L} \mathbf{v} \\
&\vdots \\
\mathbf{v}_1 &= \operatorname*{arg\,min}_{\|\mathbf{v}\|=1, \mathbf{v} \perp \mathbf{v}_n, \ldots, \mathbf{v}_2} \mathbf{v}^T \mathbf{L} \mathbf{v}
\end{aligned}
$$

SMALLEST LAPLACIAN EIGENVECTOR

The smallest eigenvector/singular vector $\mathbf{v}_n$ satisfies:

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

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

SECOND SMALLEST LAPLACIAN EIGENVECTOR

By Courant-Fischer, $\mathbf{v}_{n-1}$ is given by:

$$\mathbf{v}_{n-1} = \underset{\|\mathbf{v}\|=1,\ \mathbf{v}_n^T\mathbf{v}=0}{\arg\min} \ \mathbf{v}^T L\mathbf{v}$$

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

- $\mathbf{v}_{n-1}^T L\mathbf{v}_{n-1} = cut(S,T)$ as small as possible given that $\mathbf{v}_{n-1}^T\mathbf{1} = |T| - |S| = 0$.
- $\mathbf{v}_{n-1}$ would indicate the smallest perfectly balanced cut.

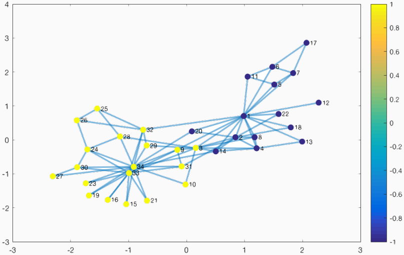
$\mathbf{v}_{n-1} \in \mathbb{R}^n$ is not generally binary, but still satisfies a 'relaxed' version of this property.

CUTTING WITH THE SECOND LAPLACIAN EIGENVECTOR

Find a good partition of the graph by computing

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

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



CUTTING WITH THE SECOND LAPLACIAN EIGENVECTOR

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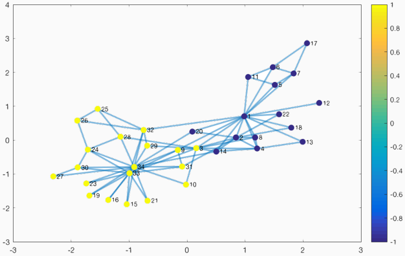
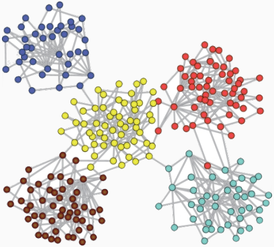


SPECTRAL PARTITIONING IN PRACTICE

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

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

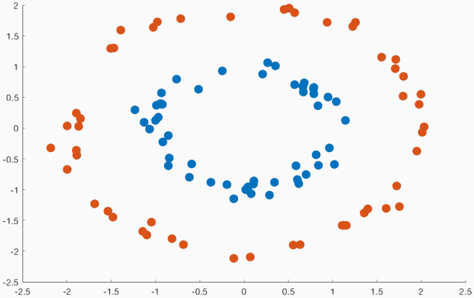


Spectral Clustering:

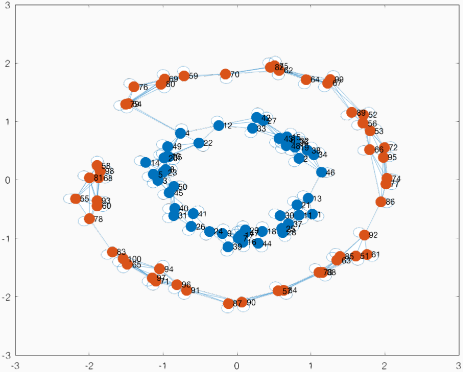
- Compute smallest k eigenvectors $\mathbf{v}_{n-1}, \ldots, \mathbf{v}_{n-k}$ of $\mathbf{L}$.
- Represent each node by its corresponding row in $\mathbf{V} \in \mathbb{R}^{n \times k}$ whose rows are $\mathbf{v}_{n-1}, \ldots \mathbf{v}_{n-k}$.
- Cluster these rows using k-means clustering (or really any clustering method).

LAPLACIAN EMBEDDING

Original Data: (not linearly separable)

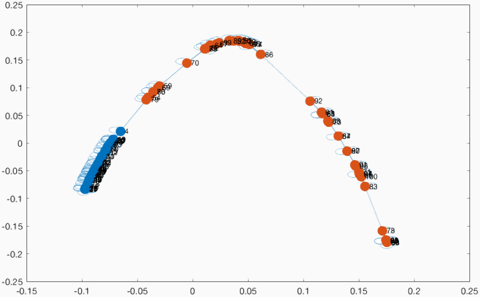


k-Nearest Neighbors Graph:



LAPLACIAN EMBEDDING

Embedding with eigenvectors v_{n-1}, v_{n-2}: (linearly separable)



GENERATIVE MODELS

So far: Showed that spectral clustering partitions a graph along a small cut between large pieces.

- No formal guarantee on the 'quality' of the partitioning.
- Would be difficult to analyze for general input graphs.

Common approach: Give a natural generative model for which produces random but realistic 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

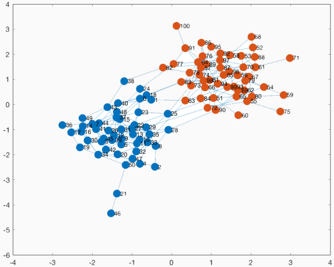
Ideas for a generative model for graphs that would allow us to understand partitioning?

STOCHASTIC BLOCK MODEL

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.

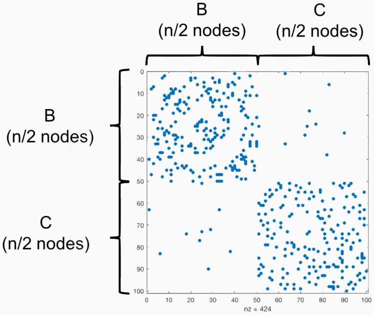
- Any two nodes in the same group are connected with probability p (including self-loops).
- Any two nodes in different groups are connected with prob. $q < p$.



LINEAR ALGEBRAIC VIEW

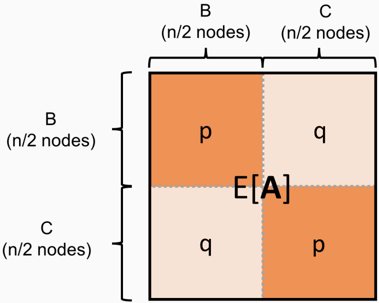
Let G be a stochastic block model graph drawn from $G_n(p, q)$.

- Let $\mathbf{A} \in \mathbb{R}^{n \times n}$ be the adjacency matrix of G. What is $\mathbb{E}[\mathbf{A}]$?



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.

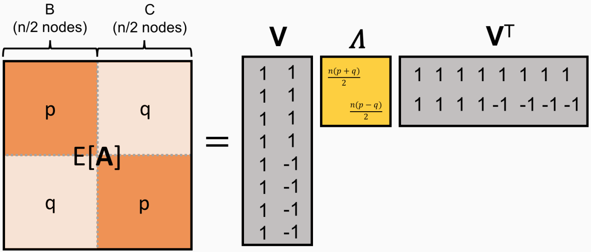


What are the eigenvectors and eigenvalues of $\mathbb{E}[\mathbf{A}]$?

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

EXPECTED ADJACENCY SPECTRUM



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

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

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

EXPECTED LAPLACIAN SPECTRUM

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

- If the random graph G (equivilantly $\mathbf{A}$ and $\mathbf{L}$) were exactly equal to its expectation, partitioning using this eigenvector would exactly recover communities B and C.

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 machine learning.

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

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.

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 $\mathsf{A}, \overline{\mathsf{A}} \in \mathbb{R}^{d\times d}$ are symmetric with $\|\mathsf{A} - \overline{\mathsf{A}}\|_2 \leq \epsilon$ 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 $\overline{\mathsf{A}}$.

The error gets larger if there are eigenvalues with similar magnitudes.

EIGENVECTOR PERTURBATION

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

APPLICATION TO STOCHASTIC BLOCK MODEL

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

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

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

$$\sin\theta(v_2, \bar{v}_2) \leq \frac{O(\sqrt{pn})}{\min_{j\neq i}|\lambda_i - \lambda_j|} \leq \frac{O(\sqrt{pn})}{(p-q)n/2} == O\left(\frac{\sqrt{p}}{(p-q)\sqrt{n}}\right)$$

Recall: $\mathbb{E}[\mathbf{A}]$, has eigenvalues $\lambda_1 = \frac{(p+q)n}{2}$, $\lambda_2 = \frac{(p-q)n}{2}$, $\lambda_i = 0$ for $i \geq 3$.

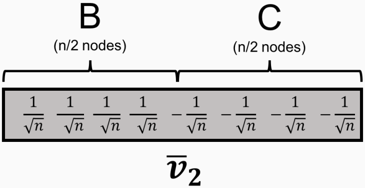
$$\min_{j\neq i}|\lambda_i - \lambda_j| = \min\left(qn, \frac{(p-q)n}{2}\right).$$

Typically, $\frac{(p-q)n}{2}$ will be the minimum of these two gaps.

APPLICATION TO STOCHASTIC BLOCK MODEL

So Far: $\sin\theta(v_2, \bar{v}_2) \le O\left(\frac{\sqrt{p}}{(p-q)\sqrt{n}}\right)$. What does this give us?

- Can show that this implies $\|v_2 - \bar{v}_2\|_2^2 \le O\left(\frac{p}{(p-q)^2 n}\right)$ (exercise).
- $\bar{v}_2$ is $\frac{1}{\sqrt{n}}\chi_{B,C}$: the community indicator vector.



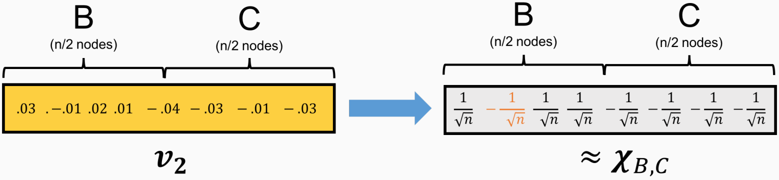
$$\begin{array}{|cccccccc|}\hline \frac{1}{\sqrt{n}} & \frac{1}{\sqrt{n}} & \frac{1}{\sqrt{n}} & \frac{1}{\sqrt{n}} & -\frac{1}{\sqrt{n}} & -\frac{1}{\sqrt{n}} & -\frac{1}{\sqrt{n}} & -\frac{1}{\sqrt{n}} \\ \hline \end{array}$$

$\bar{\boldsymbol{v}}_{\mathbf{2}}$

- Every i where $v_2(i), \bar{v}_2(i)$ differ in sign contributes $\ge \frac{1}{n}$ 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.

APPLICATION TO STOCHASTIC BLOCK MODEL

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.



B
(n/2 nodes)
C
(n/2 nodes)
$.03 \quad .-.01 \quad .02 \quad .01 \quad -.04 \quad -.03 \quad -.01 \quad -.03$
$\boldsymbol{v_2}$
B
(n/2 nodes)
C
(n/2 nodes)
$\frac{1}{\sqrt{n}} \quad -\frac{1}{\sqrt{n}} \quad \frac{1}{\sqrt{n}} \quad \frac{1}{\sqrt{n}} \quad -\frac{1}{\sqrt{n}} \quad -\frac{1}{\sqrt{n}} \quad -\frac{1}{\sqrt{n}} \quad -\frac{1}{\sqrt{n}}$
$\approx \boldsymbol{\chi_{B,C}}$

- 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.