COMPSCI 514: ALGORITHMS FOR DATA SCIENCE

Cameron Musco

University of Massachusetts Amherst. Fall 2020.

Lecture 18

LOGISTICS

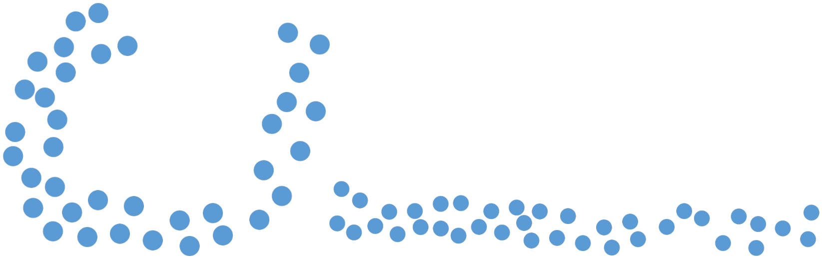
- Problem Set 3 was due yesterday.
- Solutions have been posted.
- There was no quiz due this week. Will have one due next Monday as usual.

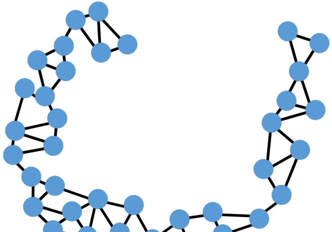
Last Class: Applications of Low-Rank Approximation

- Low-rank matrix completion (predicting missing measurements using low-rank structure).
- Entity embeddings (e.g., LSA, word embeddings). View as low-rank approximation of a similarity matrix.

Spectral Graph Theory & Spectral Clustering.

- Low-rank approximation on graph adjacency matrix for non-linear dimensionality reduction.
- Eigendecomposition to partition graphs into clusters.
- Application to the *stochastic block model* and community detection.

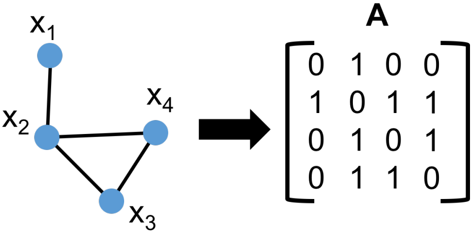




LINEAR ALGEBRAIC REPRESENTATION OF A GRAPH

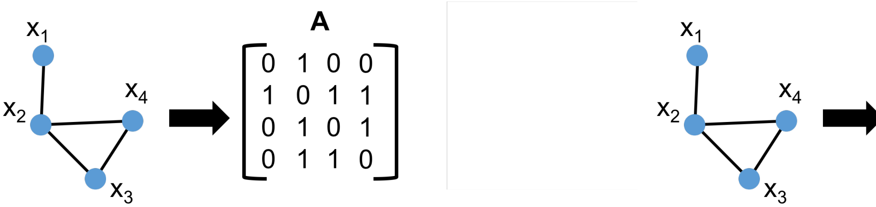
Once we have connected n data points $x_1, \ldots, x_n$ into a graph, we can represent that graph by its (weighted) adjacency matrix.

$$\mathbf{A} \in \mathbb{R}^{n \times n} \text{ with } \mathbf{A}_{i,j} = \text{ edge weight between nodes } i \text{ and } j$$



In LSA example, when $\mathbf{X}$ is the term-document matrix, $\mathbf{X}^T\mathbf{X}$ is like an adjacency matrix, where $word_a$ and $word_b$ are connected if they appear in at least 1 document together (edge weight is # documents they appear in together).

NORMALIZED ADJACENCY MATRIX



What is the sum of entries in the i^{th} column of A? The (weighted) degree of vertex i.

Often, $\mathbf{A}$ is normalized as $\bar{\mathbf{A}} = \mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2}$ where $\mathbf{D}$ is the degree matrix.

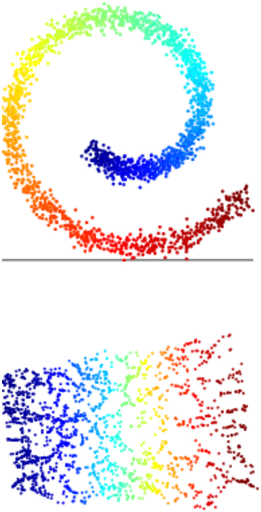
Spectral graph theory is the field of representing graphs as matrices and applying linear algebraic techniques.

ADJACENCY MATRIX EIGENVECTORS

How do we compute an optimal low-rank approximation of $\mathbf{A}$?

- Project onto the top k eigenvectors of $\mathbf{A}^T\mathbf{A} = \mathbf{A}^2$. These are just the eigenvectors of $\mathbf{A}$.

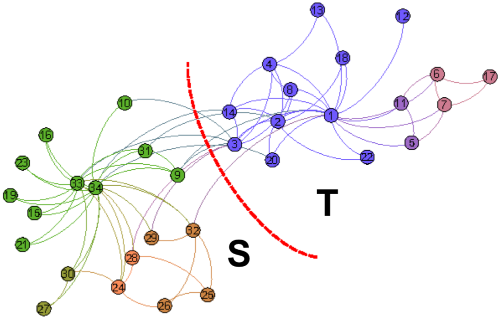
- Similar vertices (close with regards to graph proximity) should have similar embeddings.



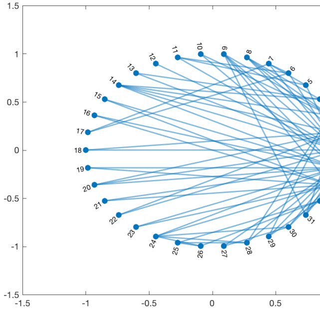
What other methods do you know for embedding or representing data points with non-linear structure?

A very common task is to partition or cluster vertices in a graph based on similarity/connectivity.

Community detection in naturally occurring networks.



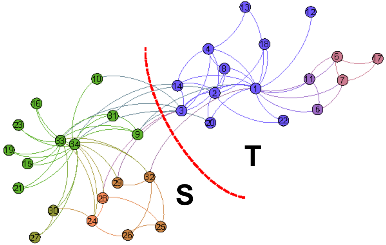
(a) Zachary Karate Club Graph



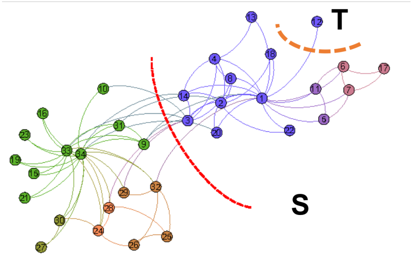
Linearly separable data

CUT MINIMIZATION

Simple Idea: Partition clusters along minimum cut in graph.



(a) Zachary Karate Club Graph



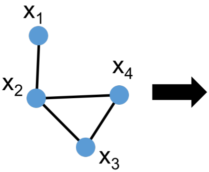
(a) Zachary Karate Club Graph

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., $\vec{v}^T\vec{1} \approx 0$.

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



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

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

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

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

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

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