COMPSCI 514: Algorithms for Data Science

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University of Massachusetts Amherst. Fall 2023.

Lecture 19

Logistics

- Problem Set 3 is due ~~Monday~~ Friday at 11:59pm.
- Office hours today in LGRC A311
- Pset 4 released Friday, Due 12/1
- Pset 5 core problems optional to replace lowest pset grade.

Summary

Last Class: SVD and Applications of Low-Rank Approximation

$X^TX \quad XX^T$

- SVD and connections to eigendecomposition and optimal low-rank approximation. $X_k = U_k U_k X = X V_k V_k^T = U_k \Sigma_k V_k^T$
- Matrix completion
- Entity Embeddings.

Summary

Last Class: SVD and Applications of Low-Rank Approximation

- SVD and connections to eigendecomposition and optimal low-rank approximation.
- Matrix completion
- Entity Embeddings.

This Class: Linear Algebraic Techniques for Graph Analysis

- Start on graph clustering for community detection and non-linear clustering.
- Spectral clustering: finding good cuts via Laplacian eigenvectors.

Spectral Clustering

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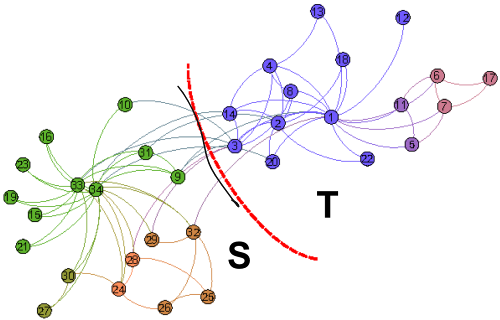
Community detection in naturally occurring networks.



(a) Zachary Karate Club Graph

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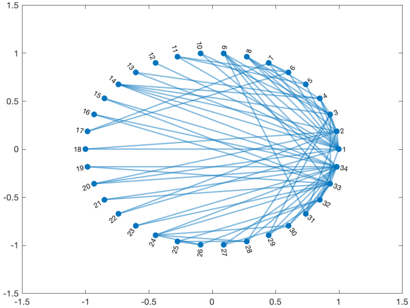

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Non-linearly separable data.

feature transfor
- non liner feature
↳ kernel methods

- graph neural networks
- neural networks

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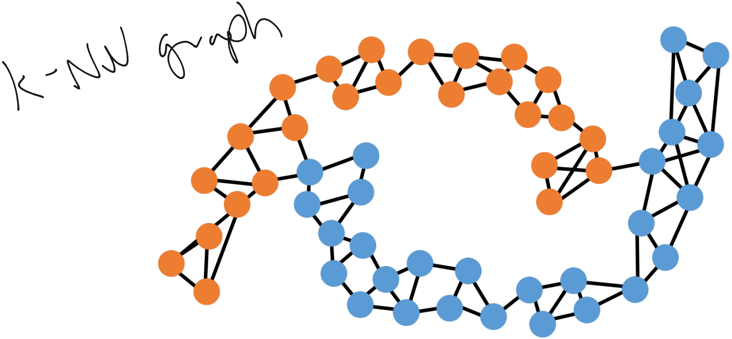

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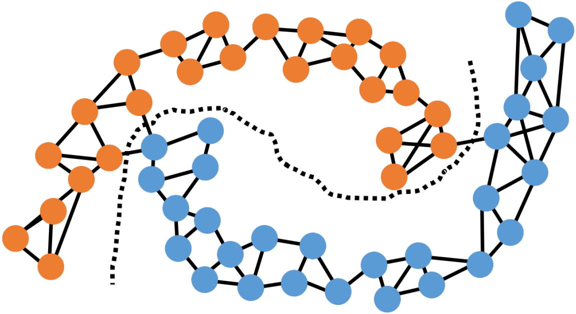

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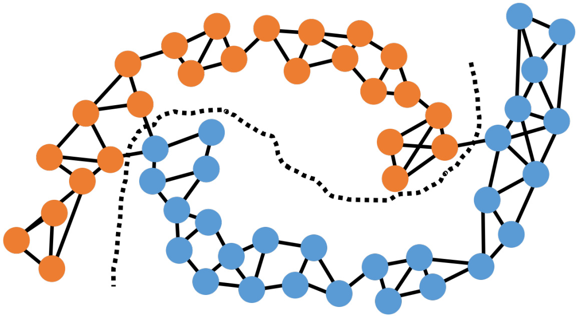
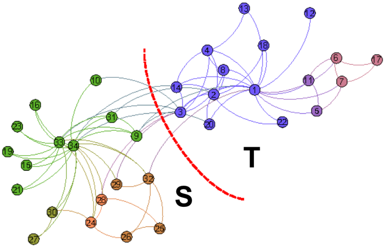


Next Few Classes: Find this cut using eigendecomposition. First – motivate why this type of approach makes sense.

Cut Minimization

Simple Idea: Partition clusters along minimum cut in graph.



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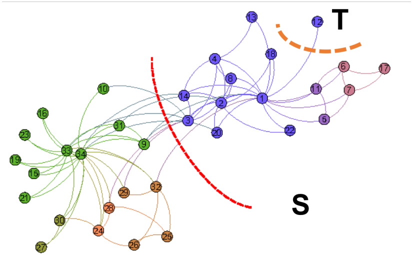

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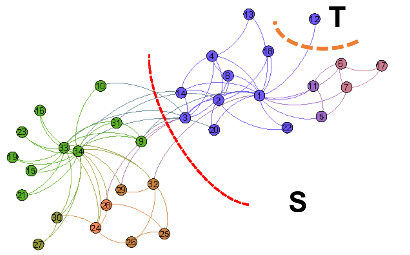

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Solution: Encourage cuts that separate large sections of the graph.

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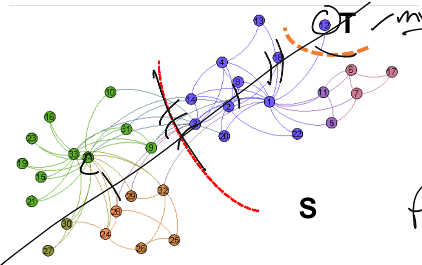

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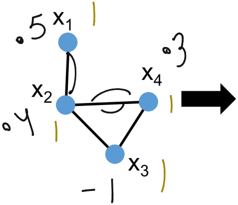
Small cuts are often not informative.

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

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



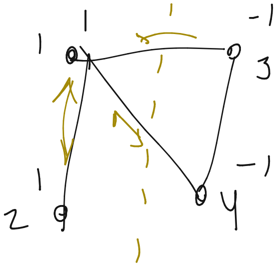
$$\underbrace{\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 2 \end{bmatrix}}_{\mathbf{D}} - \underbrace{\begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix}}_{\mathbf{A}} = \underbrace{\begin{bmatrix} 1 & -1 & 0 & 0 \\ -1 & 3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

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



$V = \begin{bmatrix} 1 \\ 1 \\ -1 \\ -1 \end{bmatrix}$

$(1-1)^2 + (1--1)^2 + (1--1)^2 + (1-1)^2 = 8$

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 $i \in T$:

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2. $\vec{v}^T \vec{1} = |T| - |S|$.

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

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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 (sort of) by eigendecomposition.

Smallest Laplacian Eigenvector

The smallest eigenvector of the Laplacian is:

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

with eigenvalue $\lambda_n(\mathbf{L}) = \vec{v}_n^T \mathbf{L} \vec{v}_n = 0$. Why?

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

Second Smallest Laplacian Eigenvector

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

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

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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:

- $\vec{v}_{n-1}^T L \vec{v}_{n-1} = \frac{4}{\sqrt{n}} \cdot cut(S, T)$ as small as possible given that $\vec{v}_{n-1}^T \vec{v}_n = \frac{1}{\sqrt{n}} \vec{v}_{n-1}^T \vec{1} = \frac{|T|-|S|}{n} = 0.$

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- I.e., $\vec{v}_{n-1}$ would indicate the smallest perfectly balanced cut.

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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.

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Cutting With the Second Laplacian Eigenvector

Find a good partition of the graph by computing

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Set S to be all nodes with $\vec{v}_{n-1}(i) < 0$, T to be all with $\vec{v}_2(i) \geq 0$.

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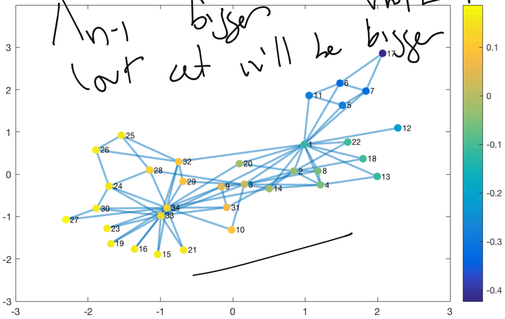

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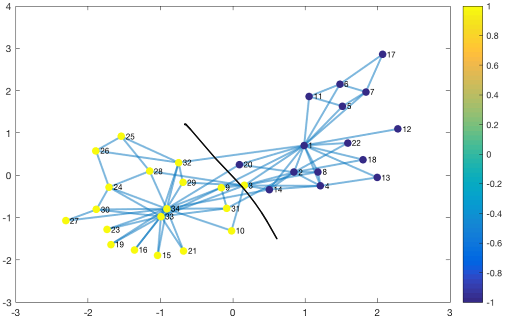

Spectral Partitioning in Practice

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

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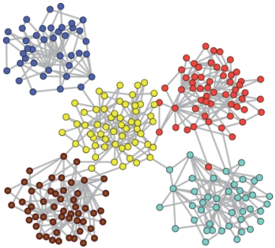

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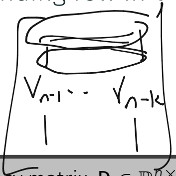

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- Cluster these rows using k-means clustering (or really any clustering method).

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Laplacian Embedding

The smallest eigenvectors of $\mathbf{L} = \mathbf{D} - \mathbf{A}$ give the orthogonal 'functions' that are smoothest over the graph. I.e., minimize

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

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Embedding points with coordinates given by $[\vec{v}_{n-1}(j), \vec{v}_{n-2}(j), \ldots, \vec{v}_{n-k}(j)]$ ensures that coordinates connected by edges have minimum total squared Euclidean distance.

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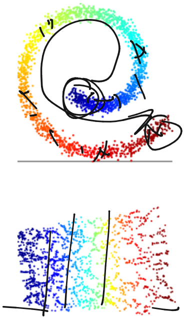
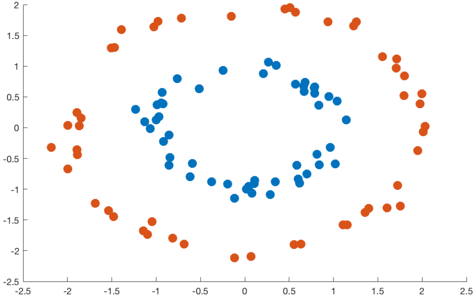


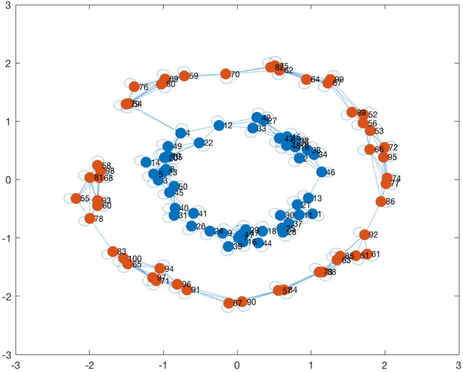
- Spectral Clustering
- Laplacian Eigenmaps
- Locally linear embedding
- Isomap
- Node2Vec, DeepWalk, etc. (variants on Laplacian)

Original Data: (not linearly separable)



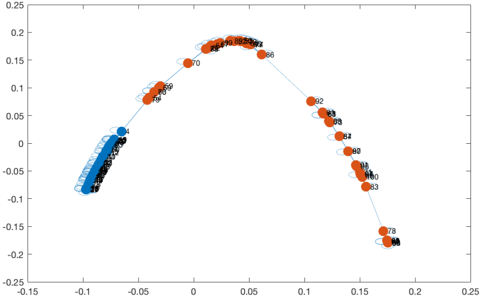
Laplacian Embedding

k-Nearest Neighbors Graph:



Laplacian Embedding

Embedding with eigenvectors $\vec{v}_{n-1}, \vec{v}_{n-2}$: (linearly separable)



So Far: Have argued that spectral clustering partitions a graph effectively, along a small cut that separates the graph into large pieces. But it is difficult to give any formal guarantee on the 'quality' of the partitioning in general graphs.

Generative Models

So Far: Have argued that spectral clustering partitions a graph effectively, along a small cut that separates the graph into large pieces. But it is difficult to give any formal guarantee on the 'quality' of the partitioning in general graphs.

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 least squares regression, k-means clustering, PCA, etc.)
- We'll do this next time, introducing the Stochastic Block Model.