COMPSCI 514: Algorithms for Data Science

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University of Massachusetts Amherst. Fall 2024.

Lecture 18

Logistics

- Problem Set 3 solutions have been posted.
- Problem Set 4 will be released soon.

Summary

Last Class: SVD and Applications of Low-Rank Approximation

$X = U\Sigma V^T$

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

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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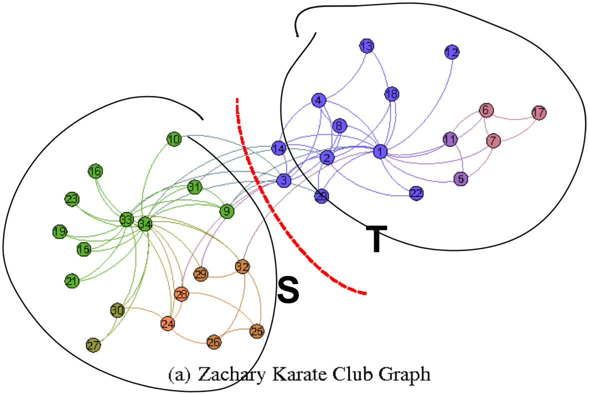

(a) Zachary Karate Club Graph

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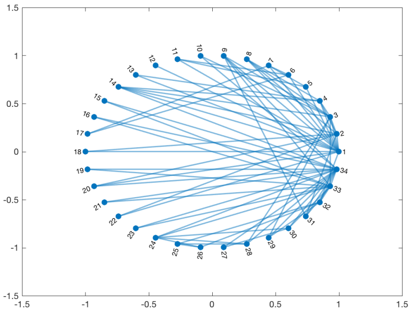

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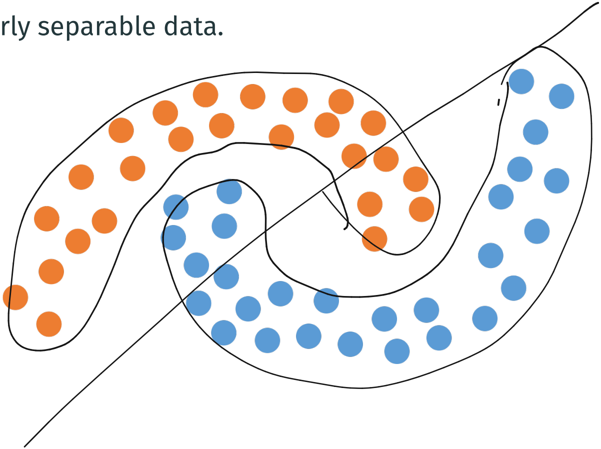
Non-linearly separable data.



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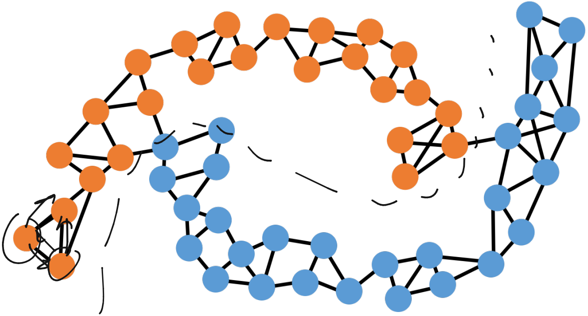

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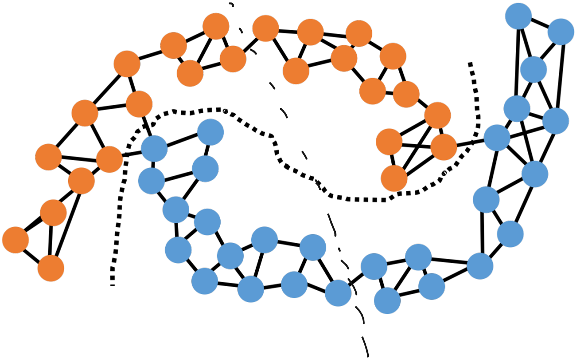

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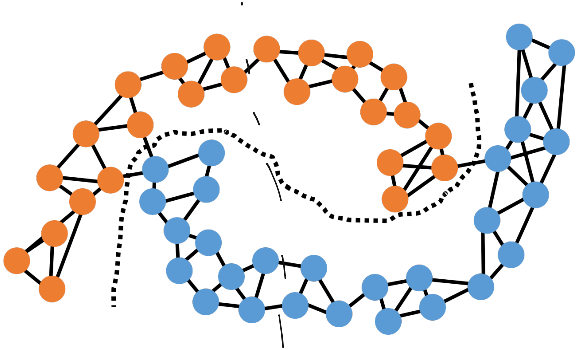
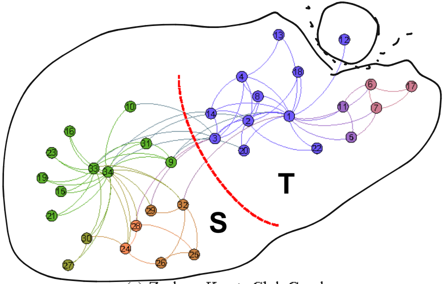


Next Few Classes: Find this cut using eigendecomposition. First – motivate why this type of approach makes sense.

Cut Minimization

Simple Idea: Partition clusters along minimum cut in graph.



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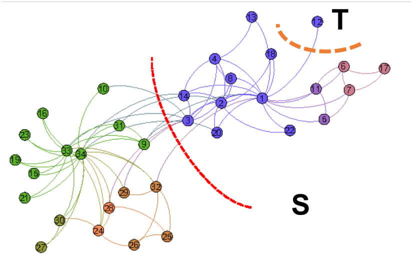

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Small cuts are often not informative.

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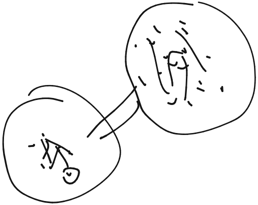

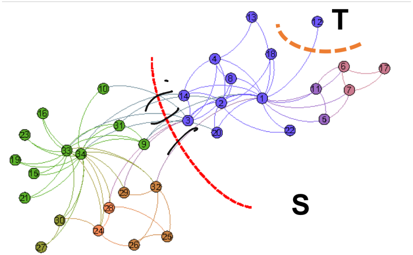

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Small cuts are often not informative.

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

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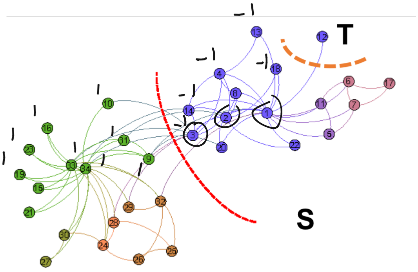
$$v = \begin{bmatrix} -1 \\ -1 \\ -1 \\ \vdots \\ 1 \\ -1 \\ 1 \end{bmatrix}$$



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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., $\sum_{i=1}^{n} v(i) =$ $\vec{v}^T\vec{1} \approx 0$.

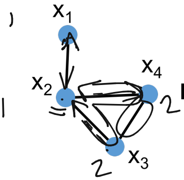
The Laplacian View

$v^T L v = 2^2 \cdot n\text{-}1 \approx 4 \cdot n$

$v^T L v = 4$

For a graph with adjacency matrix **A** and degree matrix **D**, **L** = **D** − **A** is the graph Laplacian.

$n \times n$



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

$\in \mathbb{R}^n$

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

$v \in \mathbb{R}^4$

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

$v = \begin{bmatrix} 1 \\ 1 \\ 2 \\ 2 \end{bmatrix}$

$v^T L v = 0^2 + (-1)^2 + (-1)^2 + 0^2 = 2$

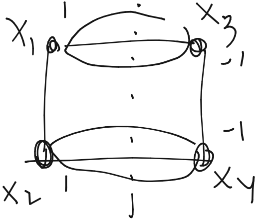
$v^T L v = 1^2 (n-1) = n-1$

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

$v^T L v = 2^2 + 2^2$

$= 8$



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

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

want both small

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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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Next Step: See how this dual minimization problem is naturally solved (sort of) by eigendecomposition.

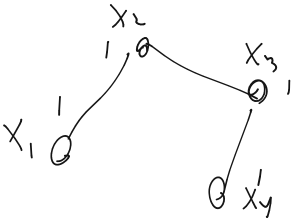
The smallest eigenvector of the Laplacian is:

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

$\lambda_1 = \max v^T L v$

$\lambda_2 = \max_{v \perp v_1} v^T L v$

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



$v = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$ $\quad v^T L v = 0$

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

Second Smallest Laplacian Eigenvector

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

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

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— cut size

perfect balance

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 $\vec{v}_{n-1}^T \vec{v}_n = \frac{1}{\sqrt{n}} \vec{v}_{n-1}^T \vec{1} = \frac{|T|-|S|}{n} = 0$.

$V_{n-1}^T V_n = 0$

$V_n = \begin{bmatrix}1\\1\\1\\1\\1\\1\end{bmatrix} \frac{1}{\sqrt{6}}$

$V_{n-1}^T 1 = 0$ $\quad [1]$

$\sum_{i=1}^{n} V_{n-1}(i) = 0$

$V_{n-1} = \begin{bmatrix}1\\1\\-1\\-1\end{bmatrix} \cdot \frac{1}{\sqrt{6}}$

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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

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

cut size

balance

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

$$\begin{bmatrix} -.58 \\ 1 \\ 0.2 \\ -.03 \\ \vdots \end{bmatrix}$$

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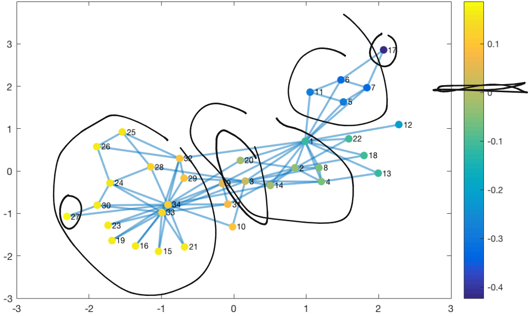

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generalize to other thresholds

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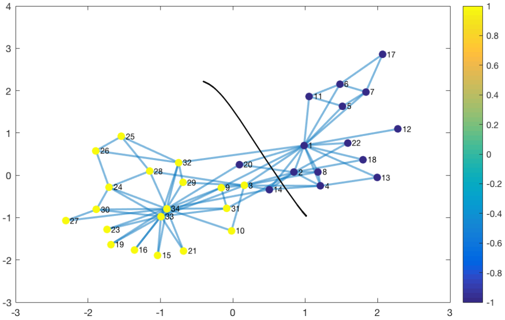

Spectral Partitioning in Practice

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

$v^T L v$

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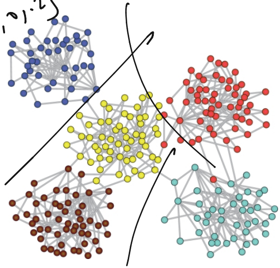
Important Consideration: What to do when we want to split the graph into more than two parts?

[.5, .03, 1, 0, .2]



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Spectral Clustering:

- Compute smallest k nonzero eigenvectors $\vec{v}_{n-1}, \ldots, \vec{v}_{n-k}$ of $\overline{\mathbf{L}}$.

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Spectral Clustering:

$k = 2$

$$\begin{array}{cc} v_{n-1} & v_{n-2} \\ \end{array}$$
$$\begin{bmatrix} -1 & .2 \\ -.7 & .03 \\ 0 & \vdots \\ .3 & \\ 1 & \end{bmatrix}$$

- Compute smallest k nonzero eigenvectors $\vec{v}_{n-1}, \ldots, \vec{v}_{n-k}$ of $\bar{\mathbf{L}}$.
- Represent each node by its corresponding row in $\mathbf{V} \in \mathbb{R}^{n \times k}$ whose columns are $\vec{v}_{n-1}, \ldots \vec{v}_{n-k}$.

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$V^T L V$

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- Represent each node by its corresponding row in $\mathbf{V} \in \mathbb{R}^{n \times k}$ whose columns are $\vec{v}_{n-1}, \ldots \vec{v}_{n-k}$.
- 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.

[2,3]

[-1,2]

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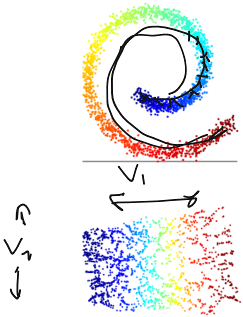


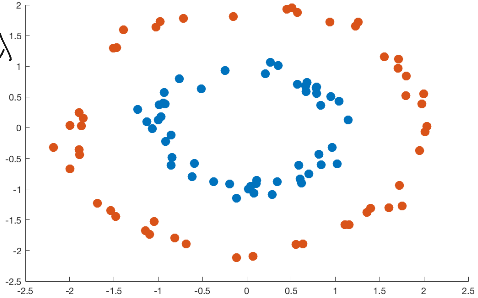
- Spectral Clustering
- Laplacian Eigenmaps
- Locally linear embedding
- Isomap
- Node2Vec, DeepWalk, etc. (variants on Laplacian)

agglomerative clustering

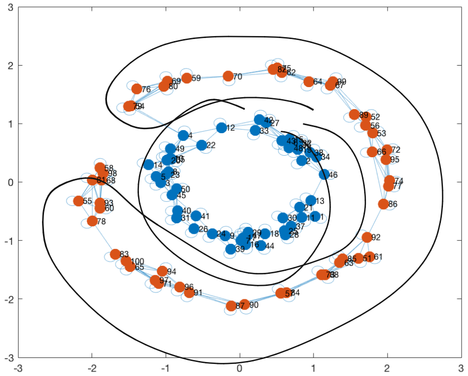
kernel method

pick the kernel

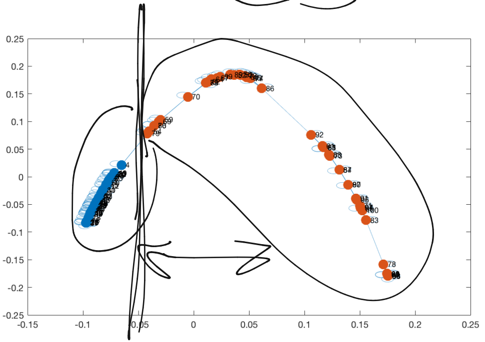
Original Data: (not linearly separable)



k-Nearest Neighbors Graph:



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



V_{n-1}

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.

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λ_{n-1}

(Fiedler value

small = well-partitioned

big = not well-partitioned

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.