COMPSCI 514: ALGORITHMS FOR DATA SCIENCE

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University of Massachusetts Amherst. Spring 2020.

Lecture 18

LOGISTICS

- Problem Set 3 is due Monday 4/13 at 8pm.

- Office hours zoom link has changed. Get from class homepage.

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.
- Start on spectral graph theory.

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- Low-rank matrix completion (predicting missing measurements using low-rank structure).
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- Start on spectral graph theory.

This Class: More Spectral Graph Theory & Spectral Clustering.

- Using eigendecomposition to partition graphs into clusters.
- Clustering non-linearly separable data.
- Application to the *stochastic block model* and community detection.

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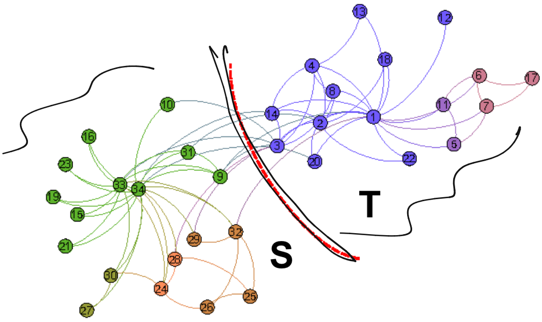
Community detection in naturally occurring networks.



(a) Zachary Karate Club Graph

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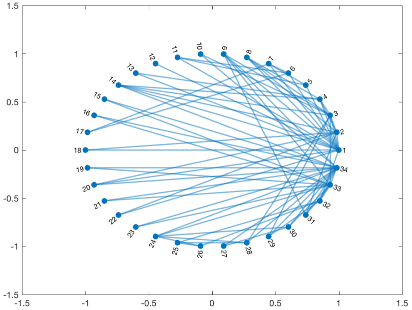
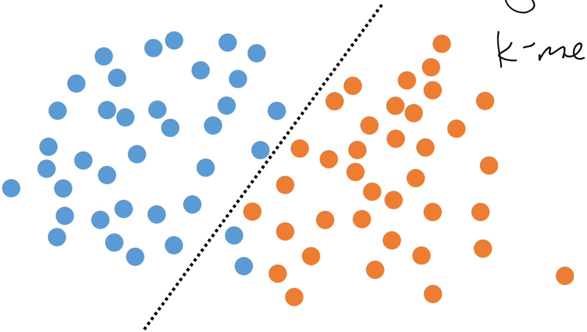


SPECTRAL CLUSTERING

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

Linearly separable data.

SVM
logistic regress.
k-means



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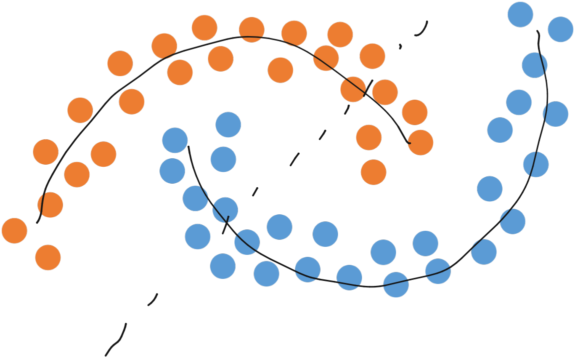
Non-linearly separable data ***k*****-nearest neighbor graph.**



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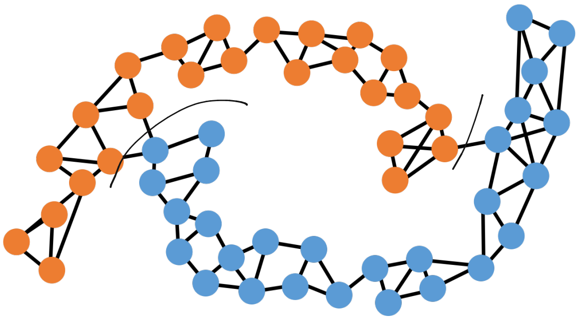

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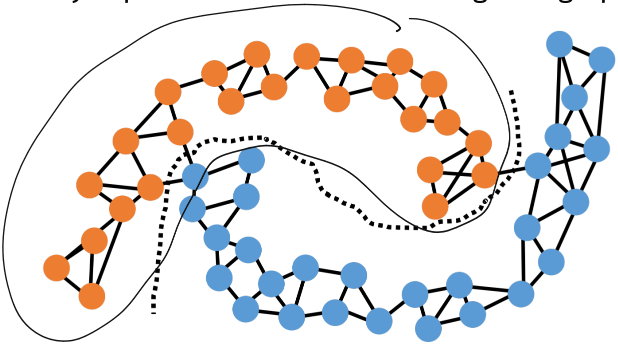

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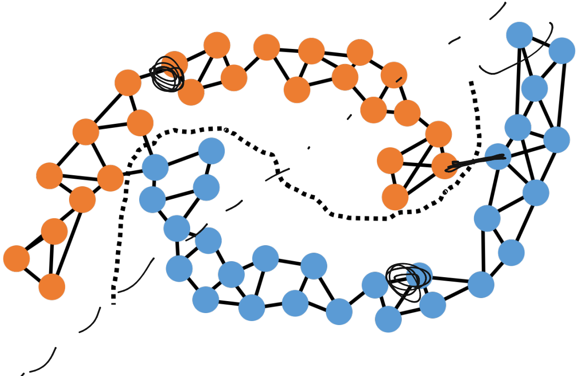
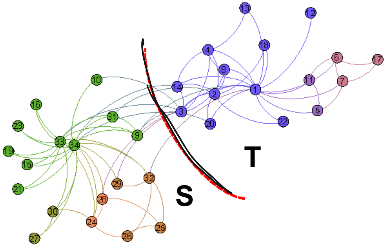


This Class: Find this cut using eigendecomposition. First – motivate why this type of approach makes sense.

Simple Idea: Partition clusters along minimum cut in graph.



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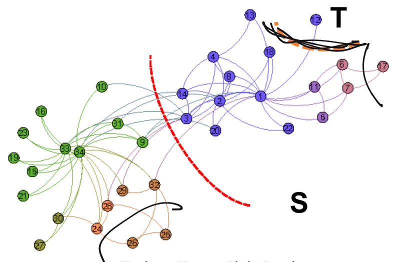

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Small cuts are often not informative.

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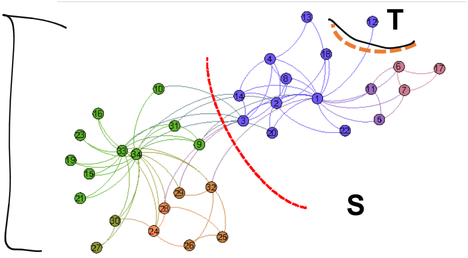

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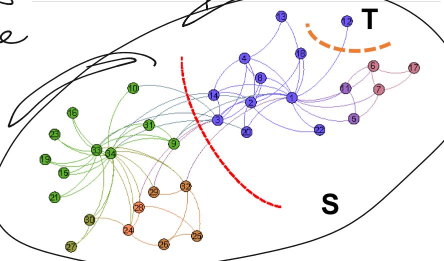
balanced min-cut.

Small cuts are often not informative.

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

Simple Idea: Partition clusters along minimum cut in graph.

2 partitions clusters have roughly equal size



(a) Zachary Karate Club Graph

$\sum_{i=1}^{n} v(i) = |S| - |T|$

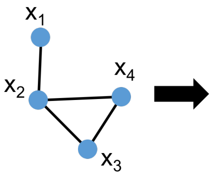
Small cuts are often not informative.

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

THE LAPLACIAN VIEW

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



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

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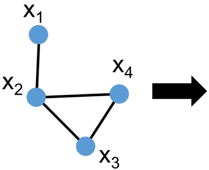

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For any vector $\vec{v}$,

$d(i)\,v(i)^2$ 0 when i & j aren't connected

$$\vec{v}^T L \vec{v} = \vec{v}^T D \vec{v} - \vec{v}^T A \vec{v} = \sum_{i=1}^{n} d(i)\vec{v}(i)^2 - \sum_{i=1}^{n}\sum_{j=1}^{n} A(i,j)\cdot v(i)\cdot v(j)$$

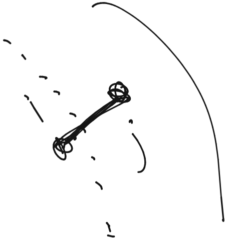
note i appears in d(i) different edges

$$= \sum_{(i,j)\in E} v(i)^2 + v(j)^2 - 2v(i)v(j) = \sum_{(i,j)\in E} [v(i) - v(j)]^2$$

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 $i \in T$:

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



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

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

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

SMALLEST LAPLACIAN EIGENVECTOR

$v_1 \dots \dots v_n \qquad \lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$

The smallest eigenvector of the Laplacian is:

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

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

$$\lambda_n = \sum_{i,j \in E} \left[v_n(i) - v_n(j) \right]^2 = 0$$

$$\begin{bmatrix} \frac{1}{\sqrt{n}} \\ \frac{1}{\sqrt{n}} \\ \vdots \\ \frac{1}{\sqrt{n}} \end{bmatrix} \qquad \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} \frac{1}{\sqrt{n}}$$

Laplacian is positive semidefinite

$\Downarrow$

all nonnegative eigenvalues

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

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$$\lambda_n = \sum_{i,j \in E} [v_n(i) - v_n(j)]^2$$

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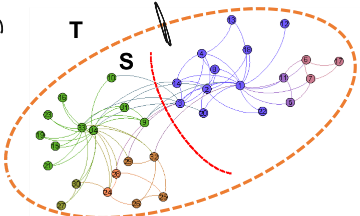

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By Courant-Fischer, the second smallest eigenvector is given by:

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

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

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

$V_{n-1}^T V_n = 0 \rightarrow V_{n-1}^T \frac{1}{\sqrt{n}} \vec{1} = 0 \rightarrow V_{n-1}^T 1 = 0$

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SECOND SMALLEST LAPLACIAN EIGENVECTOR

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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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Find a good partition of the graph by computing

$$\vec{v}_2 = \underset{v \in \mathbb{R}^d \text{ with } \|\vec{v}\|=1,\ \vec{v}^T\vec{1}=0}{\arg\min} \vec{v}^T L \vec{v}$$

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

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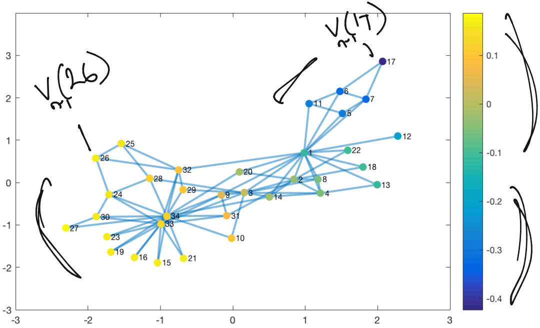

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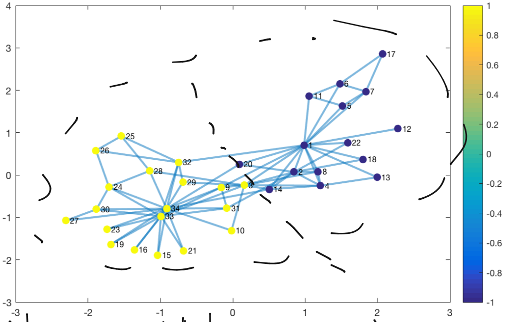
$[v_{n-1}^T 1 = 0$ — balance condition

$v^T L v$

$\Uparrow$

$[v_{n-1}^T v_n = 0$

ortho. of eigs.



orthogonality → balance cut

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

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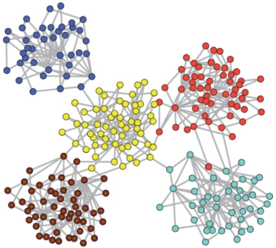
Important Consideration: What to do when we want to split the graph into more than two parts?



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Spectral Clustering:

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

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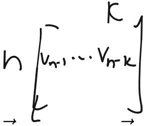

Spectral Clustering:

- 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 rows are $\vec{v}_{n-1}, \ldots \vec{v}_{n-k}$.

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- Represent each node by its corresponding row in $\mathbf{V} \in \mathbb{R}^{n \times k}$ whose rows 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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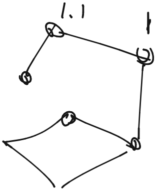
The smallest eigenvectors of $\mathbf{L} = \mathbf{D} - \mathbf{A}$ give the orthogonal ‘functions’ that are smoothest over the graph. I.e., minimize

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



LAPLACIAN EMBEDDING

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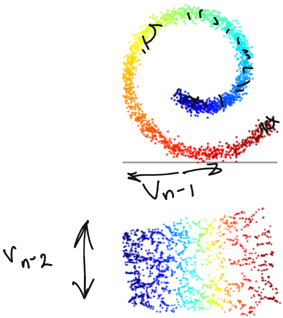
Embedding points with coordinates given by $[\vec{v}_{n-1}(j), \vec{v}_{n-2}(j), \ldots, \vec{v}_{n-k}(j)]$ ensures that coordinates connected by edges have minimum total squared Euclidean distance.

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

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

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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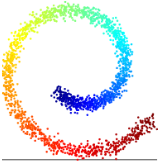
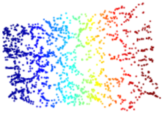
For Partitioning graphs:
1. small cut
2. balanced cut

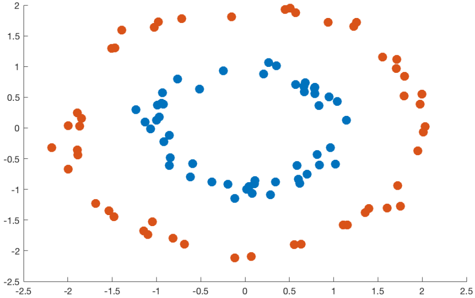
- Introduced Laplacian
- Showed that second smallest eig of L gives ~ small balanced cut → Spectral clustering



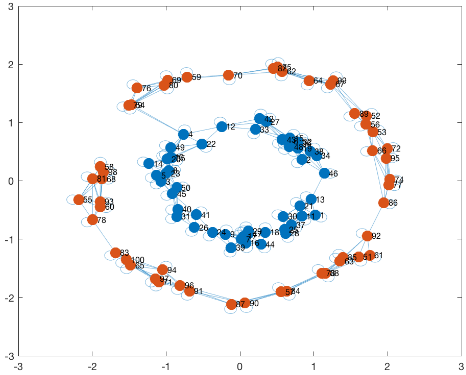


- Spectral Clustering
- Laplacian Eigenmaps
- Locally linear embedding
- Isomap
- Node2Vec, DeepWalk, etc. (variants on Laplacian)

Original Data: (not linearly separable)



k-Nearest Neighbors Graph:



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