COMPSCI 514: Algorithms for Data Science

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University of Massachusetts Amherst. Spring 2026.

Lecture 16

Logistics

- Problem Set 3 due tomorrow at 11:59pm.
- The midterm is the week after next – study material will be posted shortly.
- No quiz this week.

Summary

Last Class: Finish up SVD and Applications of Low-Rank Approximation

- Application of SVD to linear regression.
- Matrix completion
- Entity Embeddings.

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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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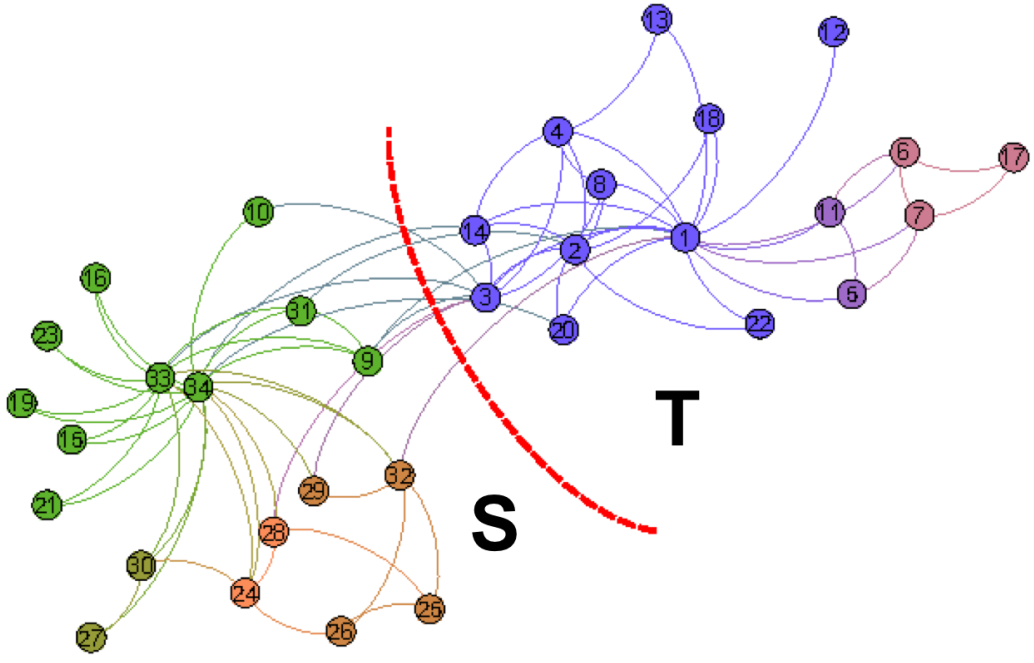
Community detection in naturally occurring networks.



(a) Zachary Karate Club Graph

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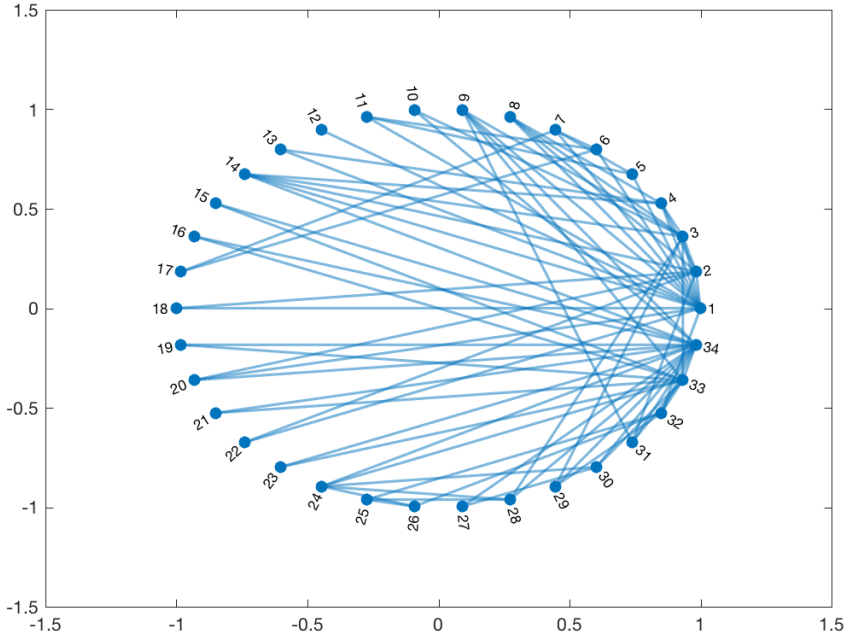

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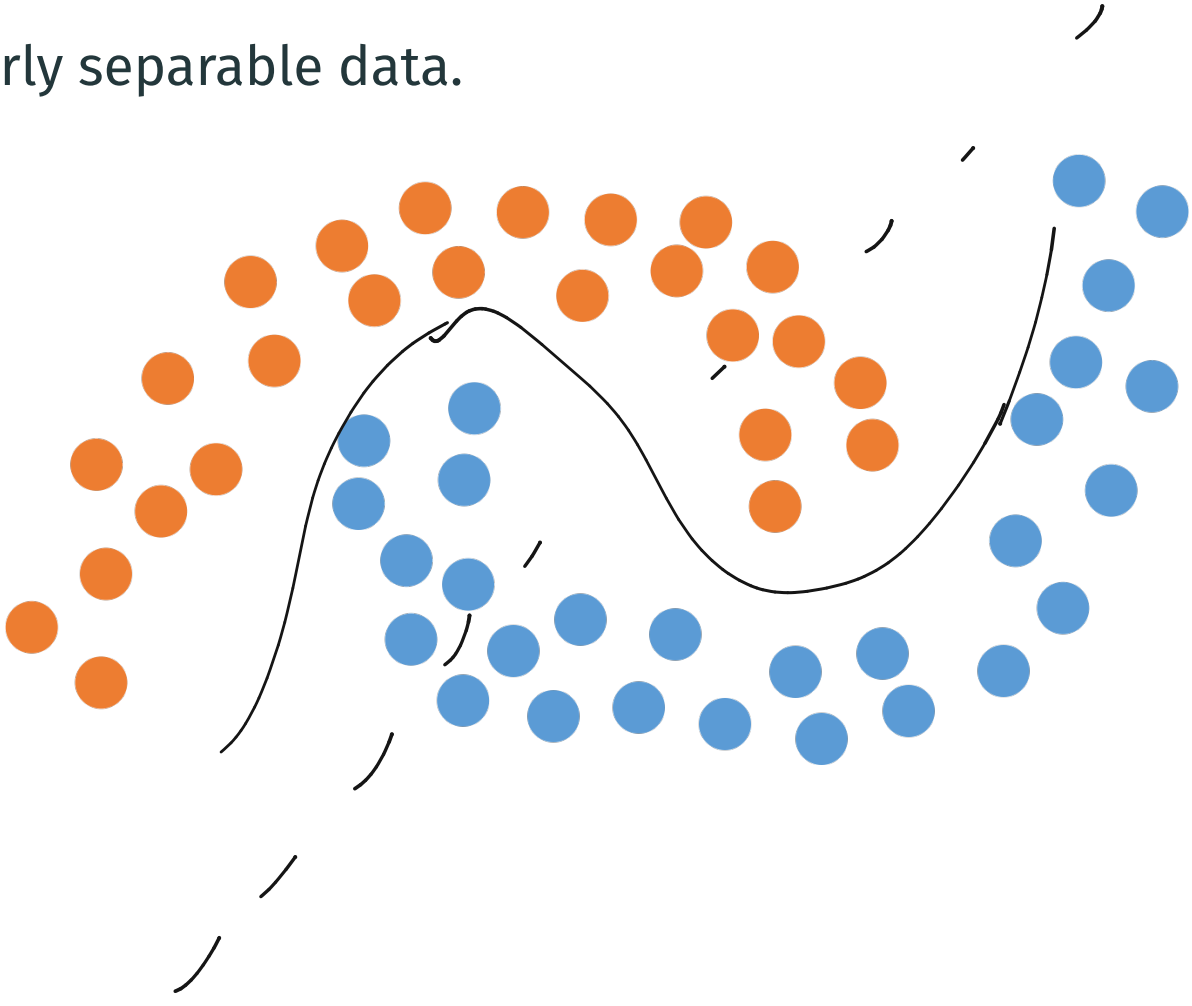
Non-linearly separable data.



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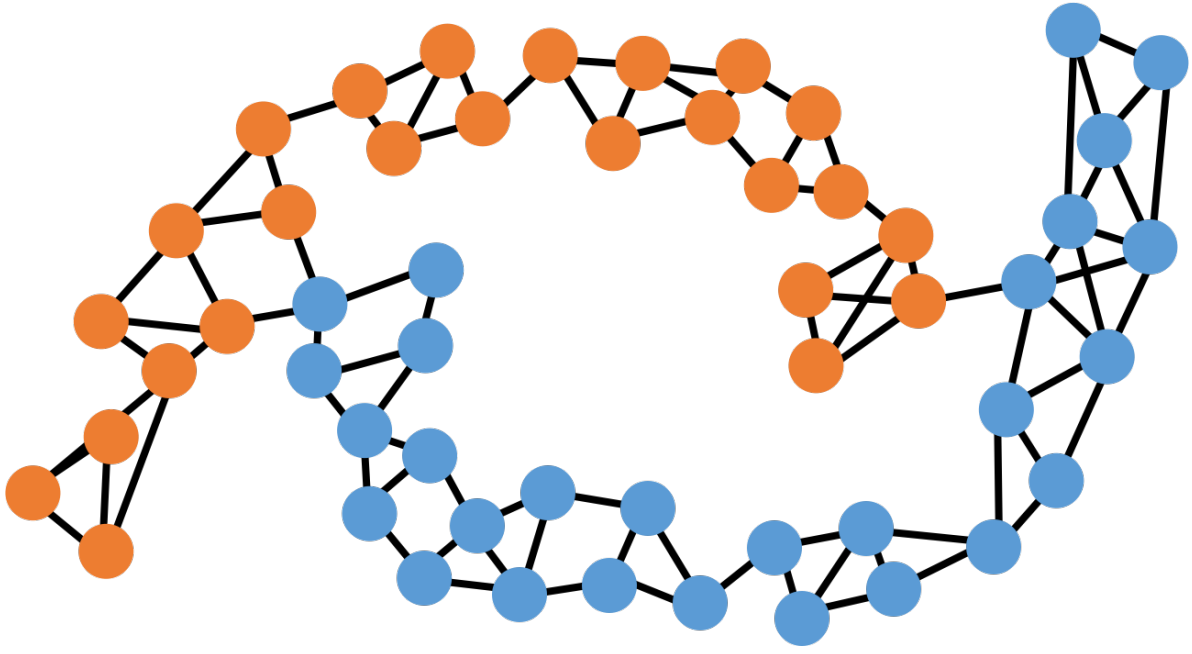
k-nearest neighbors graph



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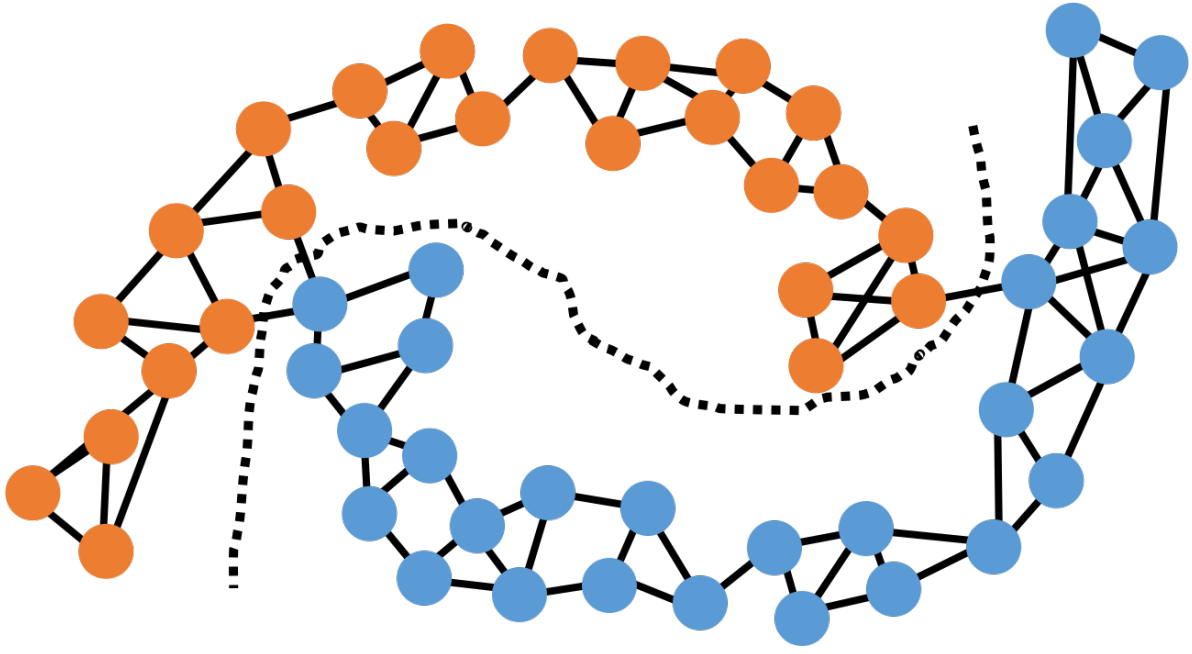

- neural networks
- decision tree
- kernel methods (support vector machine)

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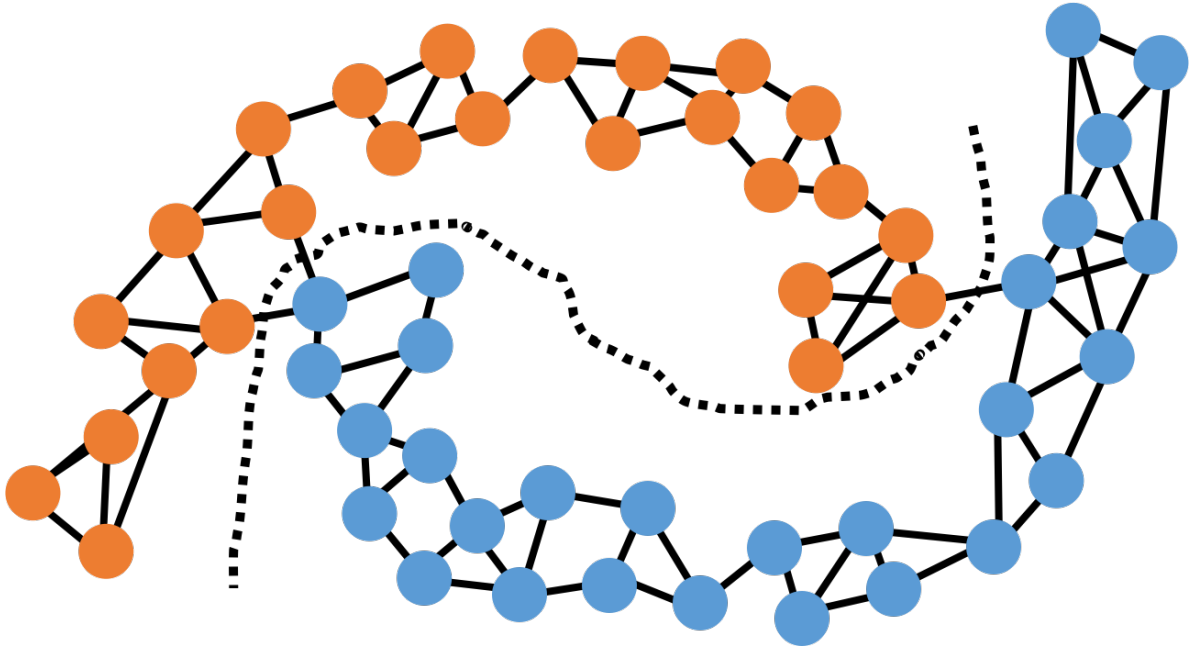
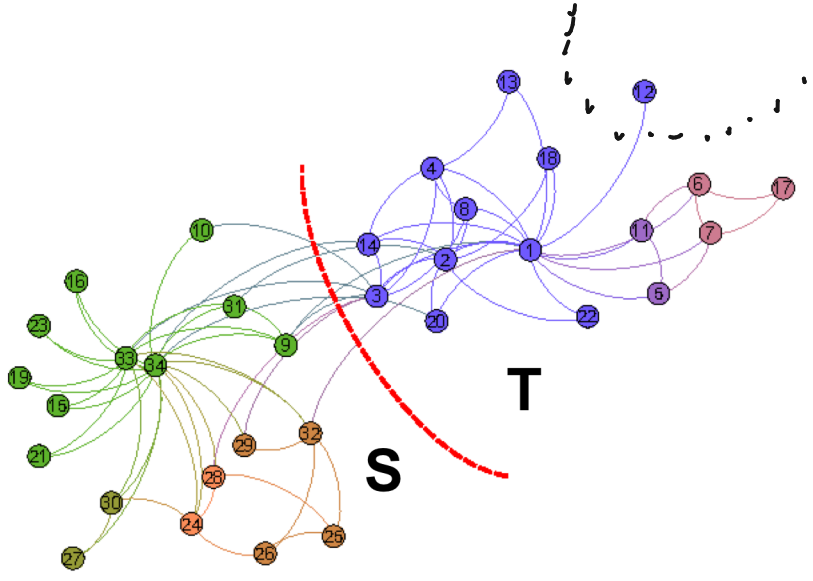


Next Few Classes: Find this cut using eigendecomposition. First – motivate why this type of approach makes sense.

Cut Minimization

Simple Idea: Partition clusters along minimum cut in graph.



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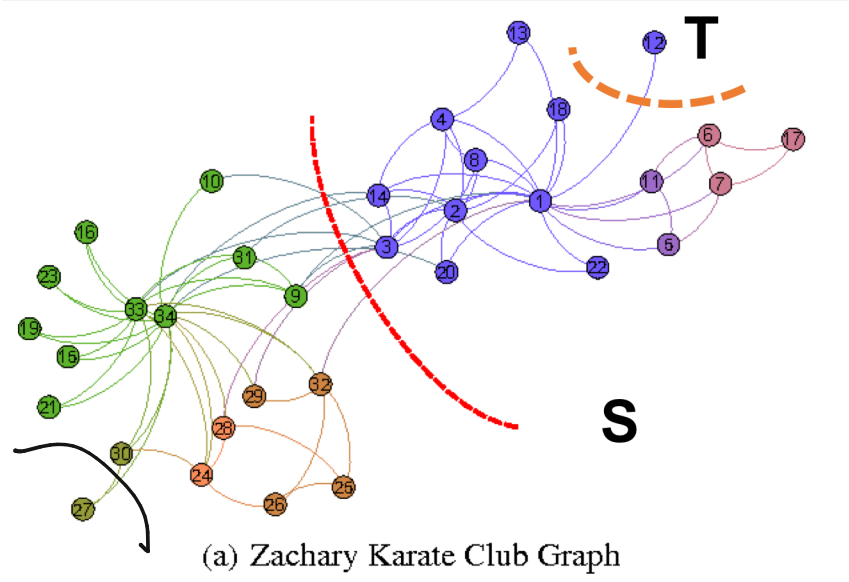

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Small cuts are often not informative.

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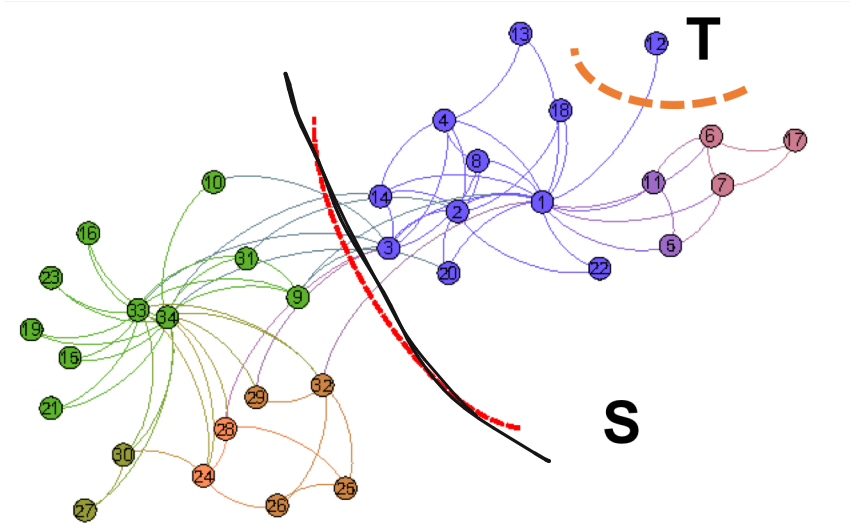

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Solution: Encourage cuts that separate large sections of the graph.

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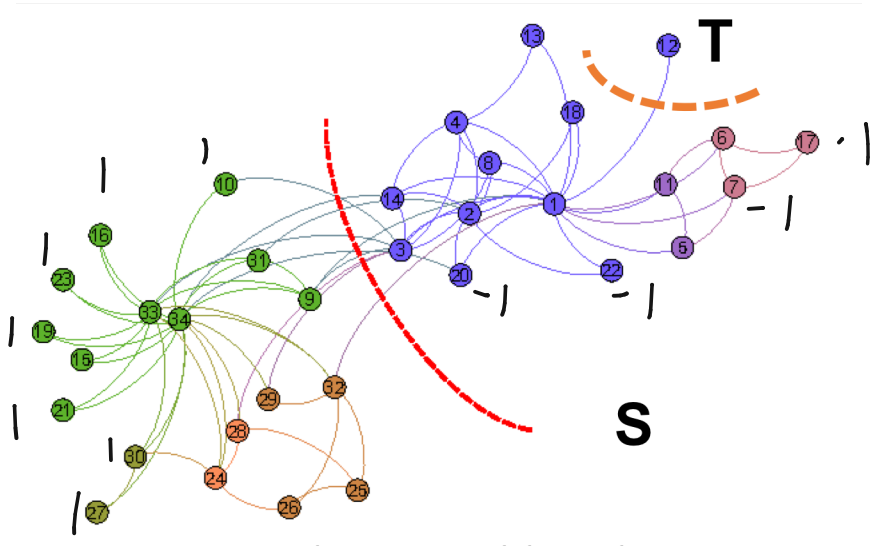

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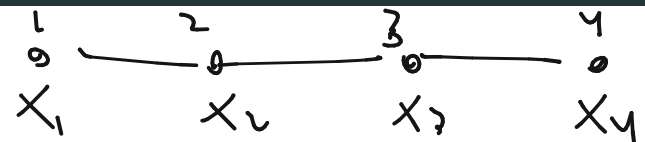
spectral graph theory

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

The Laplacian View



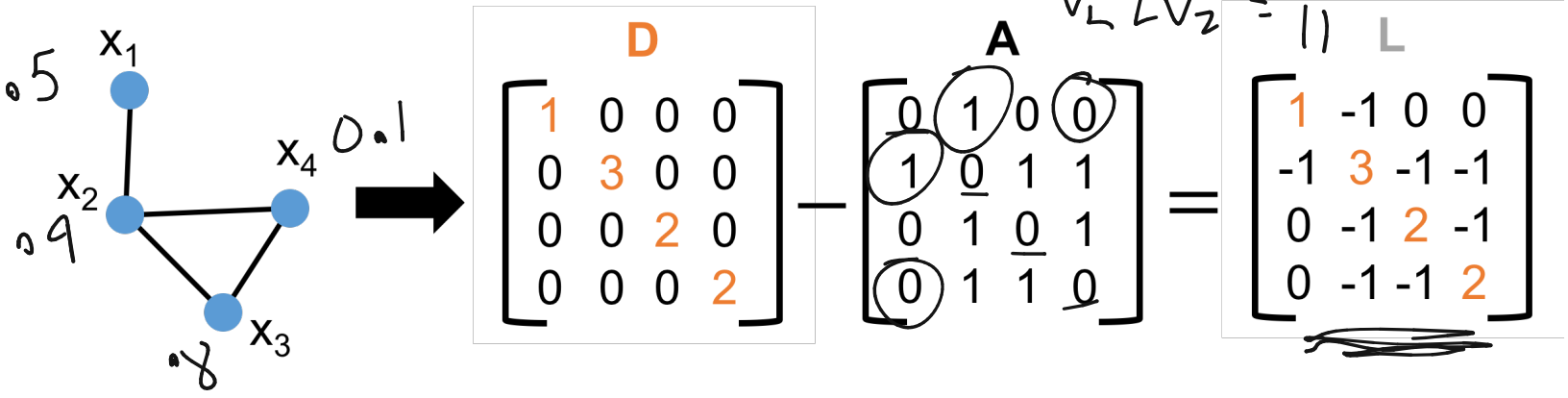
$V_1 = [1, 2, 3, 4]$

$V_2 = [1, 4, 3, 2]$

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

$V_1^T L V_1 = \sum_{(i,j)\in E} (V(i) - V(j))^2 = 3$

$V_2^T L V_2 = 11$



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

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

$V = \begin{bmatrix} 1 \\ 2 \\ 0 \\ 1 \end{bmatrix}$

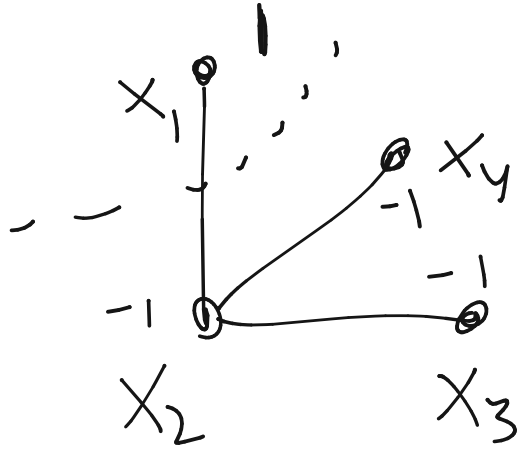
$(1-2)^2 + (2-0)^2 + (2-1)^2 + (0-1)^2$

$= 7$

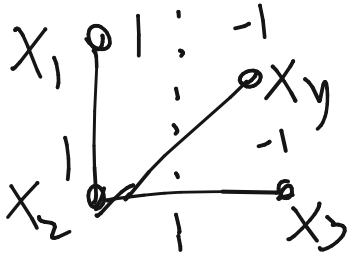
The Laplacian View

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



$v^T L v = 4 + 0 + 0 = 4$



$v^T L v = 0 + 4 + 4 = 8$

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

cutsize

balance

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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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$$\sum_{i=-1} v(i) = |T| \cdot 1 + |S| \cdot -1 = |T| - |S|$$

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 (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?

$$v^T L v = \sum_{(i,j) \in E} (v(i) - v(j))^2 = 0$$

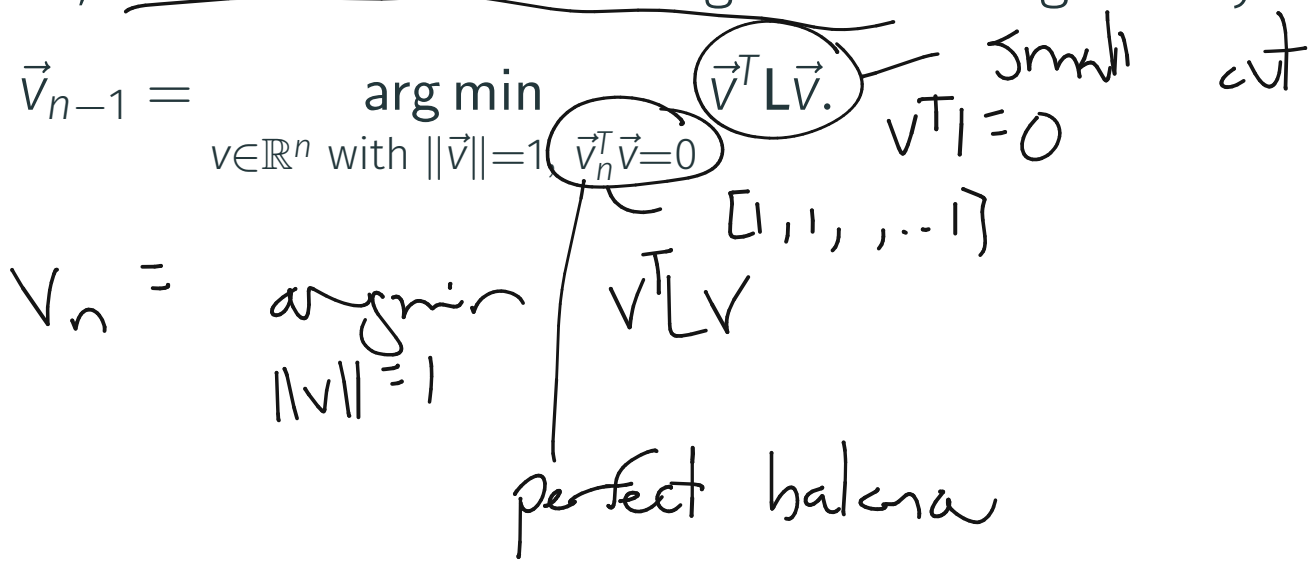
$$\begin{bmatrix} & L & \end{bmatrix} \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix} = \begin{bmatrix} & D & \end{bmatrix} \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix} - \begin{bmatrix} 0 & 1 & \cdots & 0 & 1 \\ 1 & 0 & & A & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \\ \vdots \\ d_n \end{bmatrix} - \begin{bmatrix} d_1 \\ d_2 \\ \vdots \\ d_n \end{bmatrix} = 0$$

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:

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



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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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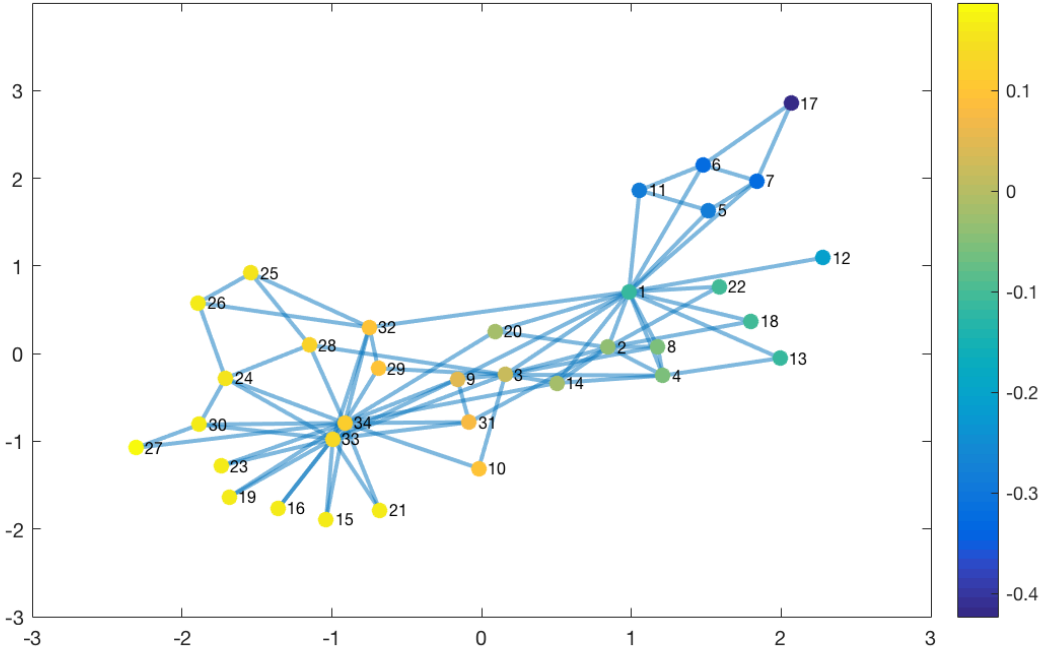
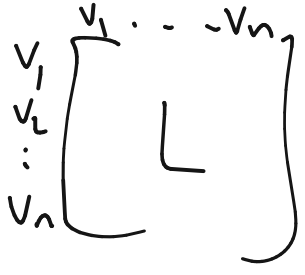
$V_{n-1} = \begin{bmatrix} .01 \\ .2 \\ -.3 \\ -.02 \\ .5 \end{bmatrix}$





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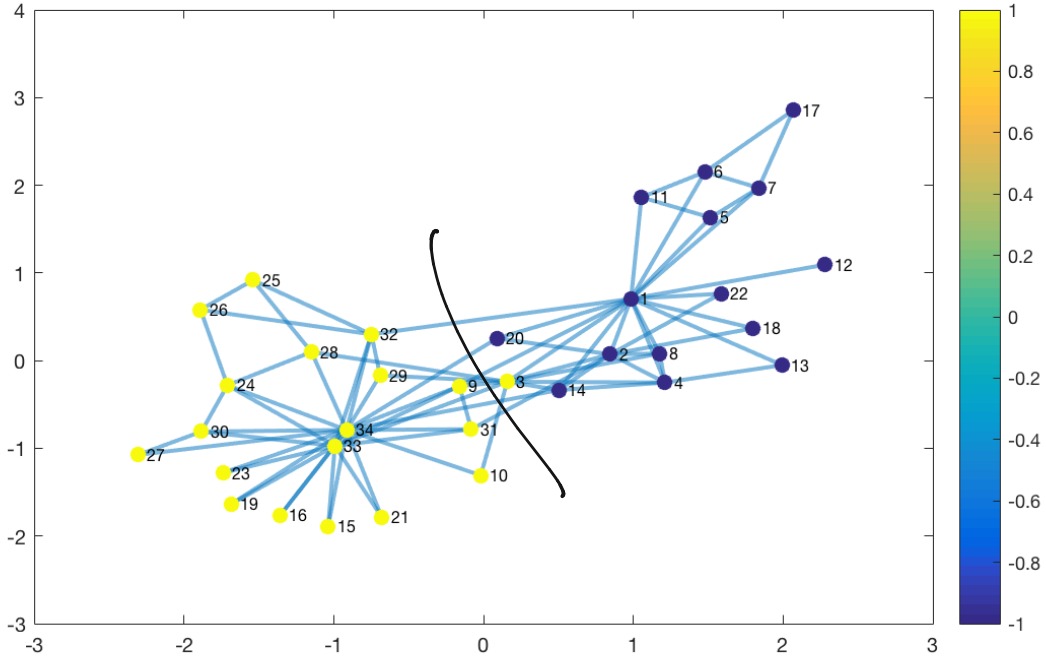
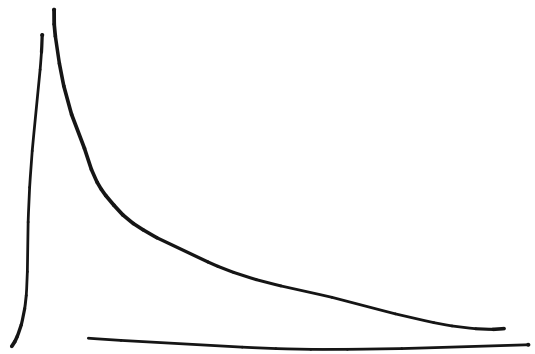


Spectral Partitioning in Practice

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

$$= D^{-1/2} D D^{-1/2} - D^{-1/2} A D^{-1/2}$$

$$I - D^{-1/2} A D^{-1/2}$$



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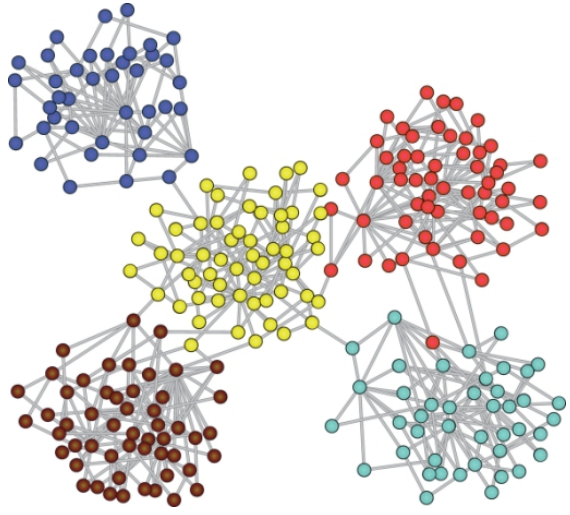
Important Consideration: What to do when we want to split the graph into more than two parts?



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Spectral Clustering:

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

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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

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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

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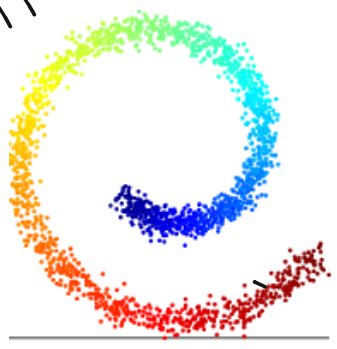
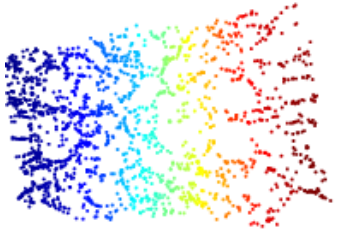
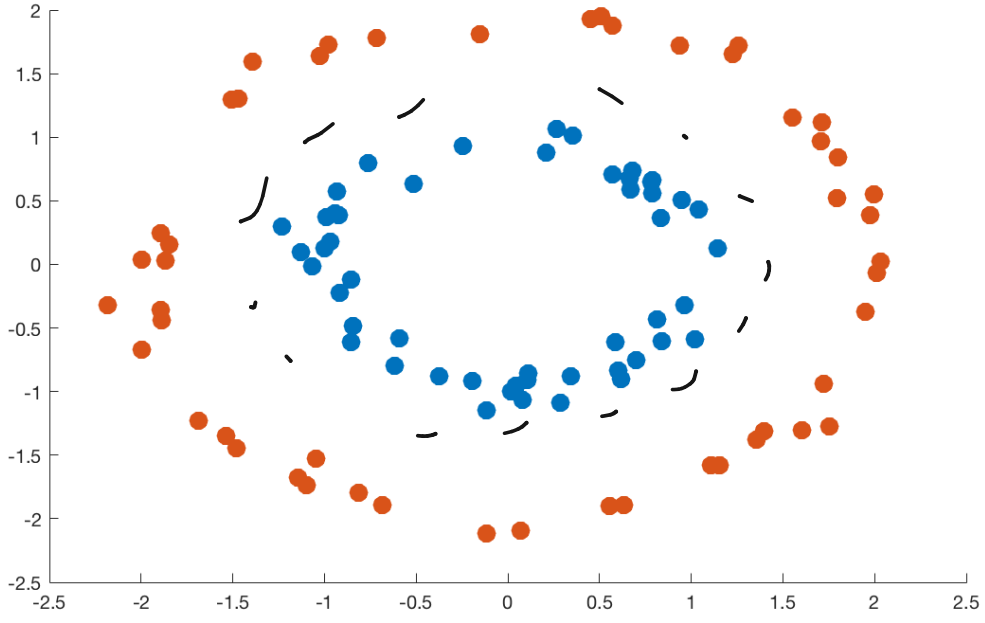




- Spectral Clustering
- Laplacian Eigenmaps
- Locally linear embedding
- Isomap
- Node2Vec, DeepWalk, etc. (variants on Laplacian)

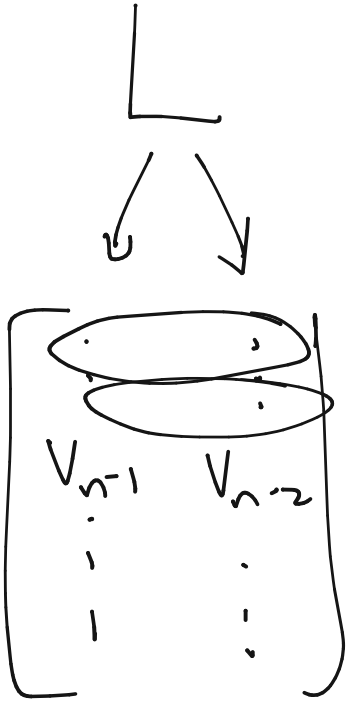
Laplacian Embedding

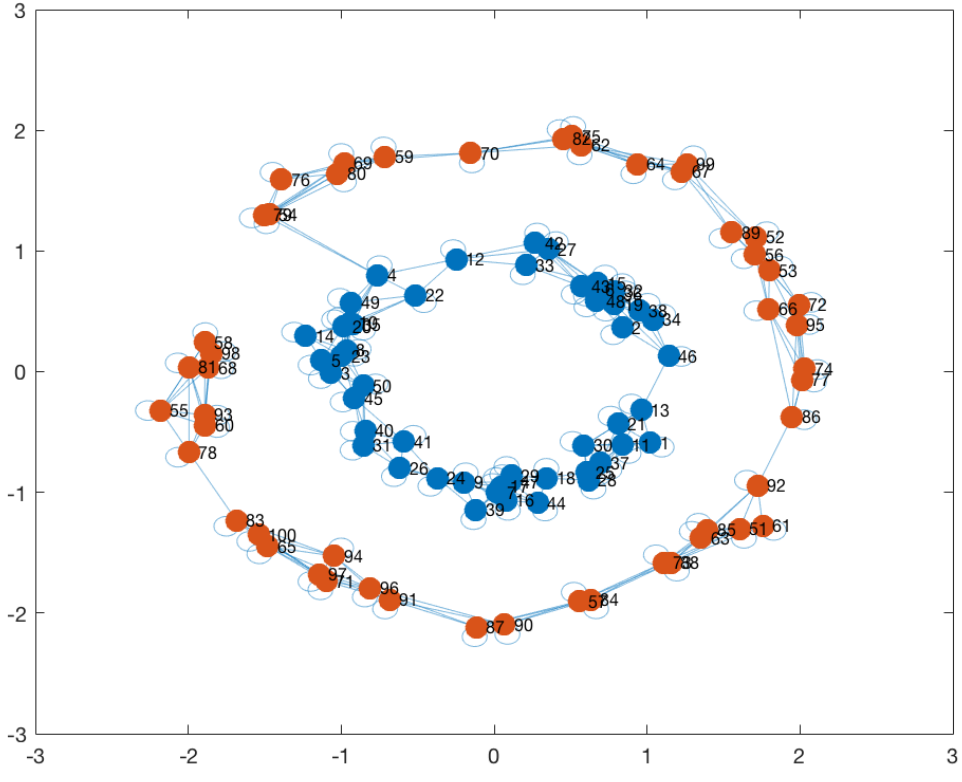
Original Data: (not linearly separable)



Laplacian Embedding

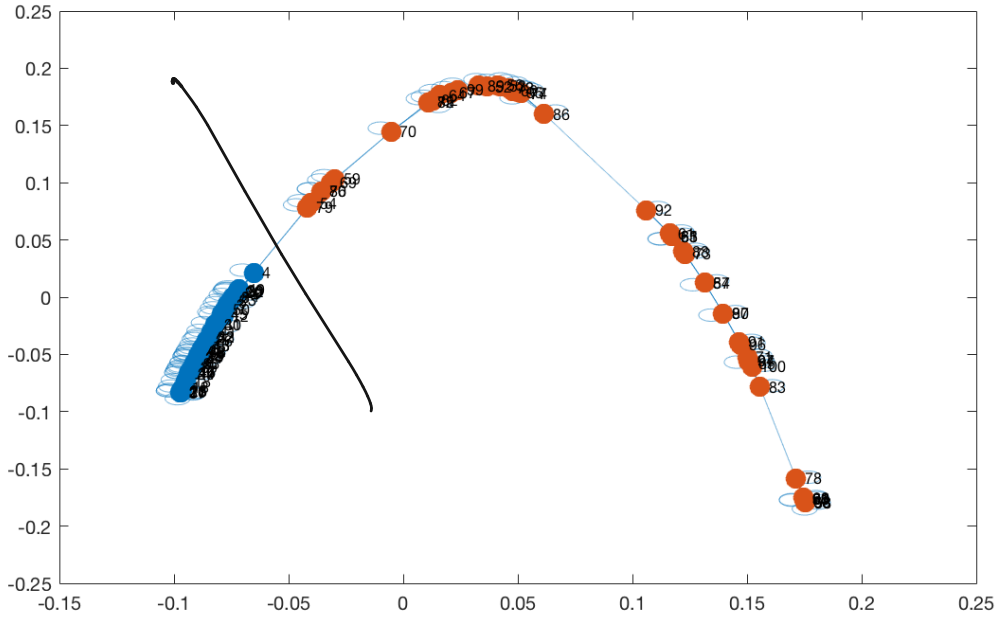
k-Nearest Neighbors Graph:





Laplacian Embedding

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



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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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.