

X Matrix Completion
X which is rank 1.

$$X = \begin{bmatrix} 1 & 2 & 3 \\ 2 & ?(4) & 26 \\ 3 & 6 & ?9 \end{bmatrix}$$

COMPSCI 514: ALGORITHMS FOR DATA SCIENCE

Cameron Musco

University of Massachusetts Amherst. Fall 2020.

Lecture 18

- 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.

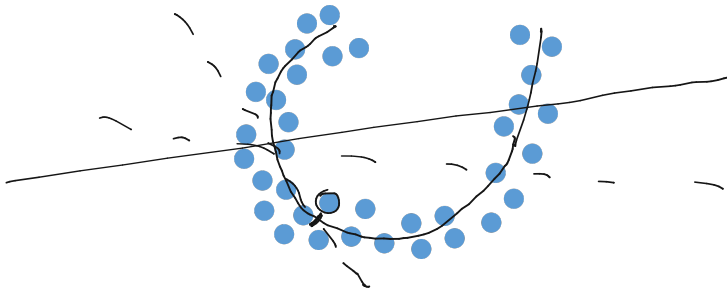
Last Class: Applications of Low-Rank Approximation

- 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.

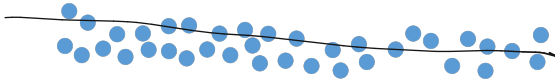
Spectral Graph Theory & Spectral Clustering.

- 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.~~

NON-LINEAR DIMENSIONALITY REDUCTION

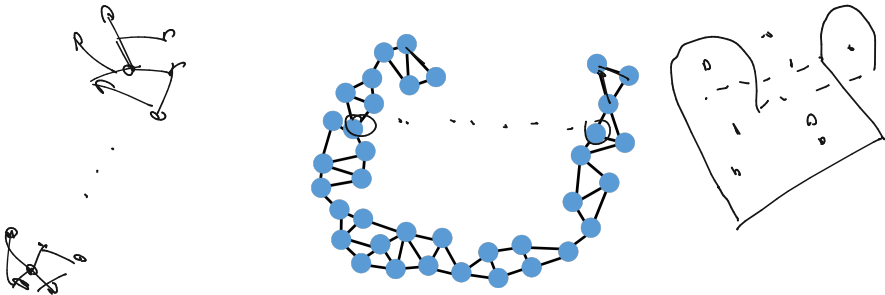


Is this set of points compressible? Does it lie close to a low-dimensional subspace? (A 1-dimensional subspace of \mathbb{R}^2 .)



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NON-LINEAR DIMENSIONALITY REDUCTION



Is this set of points compressible? Does it lie close to a low-dimensional subspace? (A 1-dimensional subspace of \mathbb{R}^d .)

A common way of automatically identifying this non-linear structure is to connect data points in a graph. E.g., a k-nearest neighbor graph.

- Connect items to similar items, possibly with higher weight edges when they are more similar.

LINEAR ALGEBRAIC REPRESENTATION OF A GRAPH

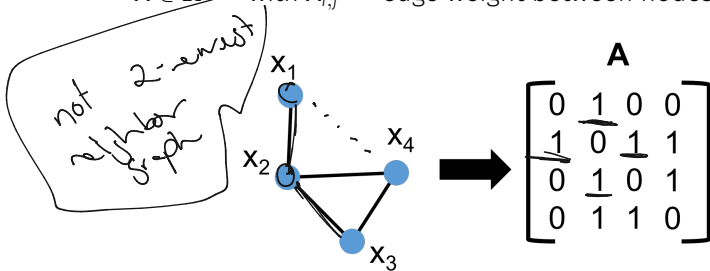
Once we have connected n data points x_1, \dots, x_n into a graph, we can represent that graph by its (weighted) adjacency matrix.

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

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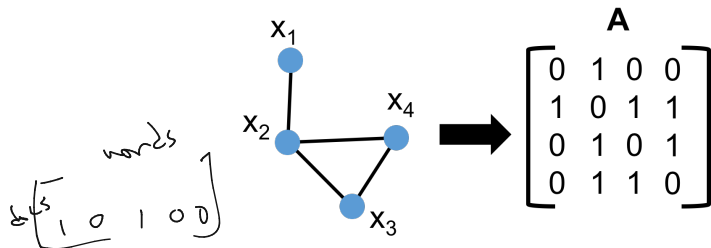
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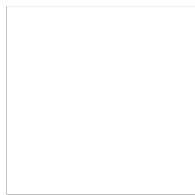
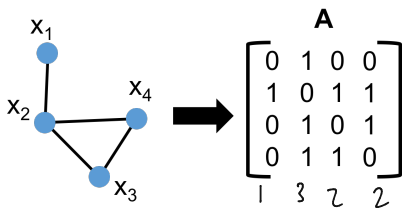
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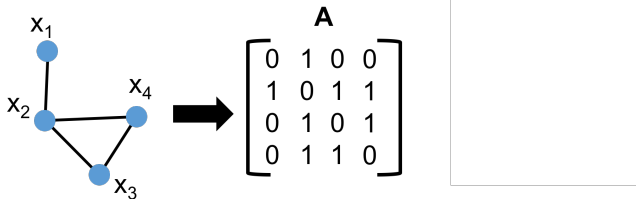
In LSA example, when X is the term-document matrix, $X^T X$ is like an adjacency matrix, where $word_a$ and $word_b$ are connected if they appear in at least 1 document together (edge weight is # documents they appear in together).

NORMALIZED ADJACENCY MATRIX



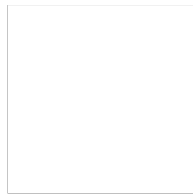
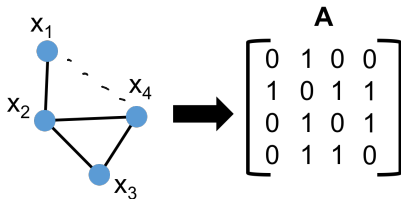
What is the sum of entries in the i^{th} column of A ?

NORMALIZED ADJACENCY MATRIX



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

NORMALIZED ADJACENCY MATRIX

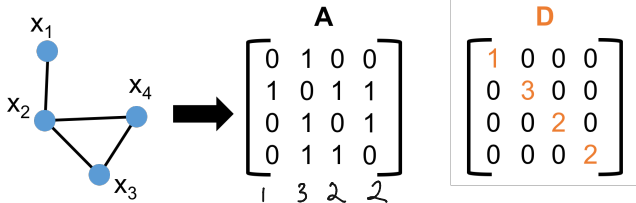


What is the sum of entries in the i^{th} column of A ? The (weighted) degree of vertex i .

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



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NORMALIZED ADJACENCY MATRIX

symmetric

$$\bar{\mathbf{A}} = \mathbf{A}\mathbf{D}^{-1/2} = \mathbf{D}^{-1/2}\mathbf{A}$$

$$\begin{bmatrix} 0 & \frac{1}{\sqrt{3}} & 0 & 0 \\ \frac{1}{\sqrt{3}} & 0 & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} \\ 0 & \frac{1}{\sqrt{6}} & 0 & \frac{1}{2} \\ 0 & \frac{1}{\sqrt{6}} & \frac{1}{2} & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{3}} & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{3}} & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{2}} \end{bmatrix}$$

What is the sum of entries in the i^{th} column of \mathbf{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.

NORMALIZED ADJACENCY MATRIX

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

ADJACENCY MATRIX EIGENVECTORS

$(X^T X)_{ab} = \#$ docs that words a & words b appear in
 How do we compute an optimal low-rank approximation of A ?

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

$$A \approx V_k \Lambda_k V_k^T$$

$$\begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} \approx \underbrace{\begin{bmatrix} V_1 & V_2 \end{bmatrix}}_Y \begin{bmatrix} \lambda_1 & & \\ & \lambda_2 & \\ & & \end{bmatrix} \underbrace{\begin{bmatrix} V_1^T \\ V_2^T \\ W^T \end{bmatrix}}_{Z^T}$$

$V \Lambda V^T \xrightarrow{V^T} \Lambda \xrightarrow{V} V \Lambda V^T$

$$\langle y^{(i)}, z^{(j)} \rangle \approx 1$$

$$\langle y^{(i)}, z^{(j)} \rangle \approx 0$$

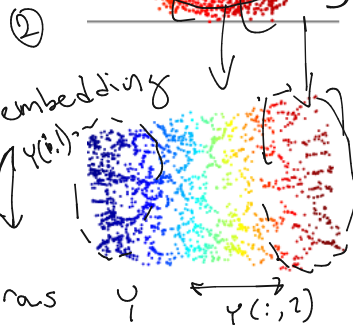
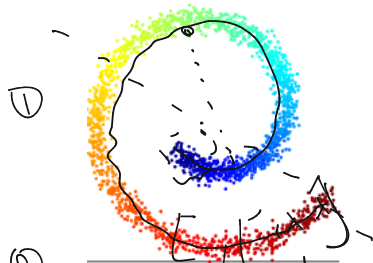
How do we compute an optimal low-rank approximation of \mathbf{A} ?

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

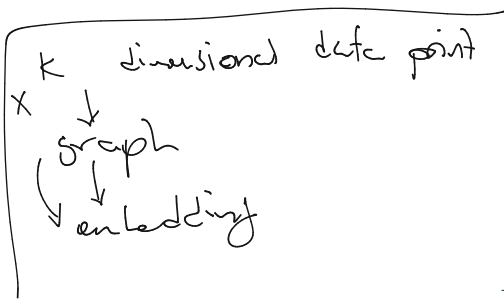
- Similar vertices (close with regards to graph proximity) should have similar embeddings.

SPECTRAL EMBEDDING

original data

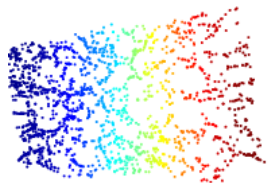
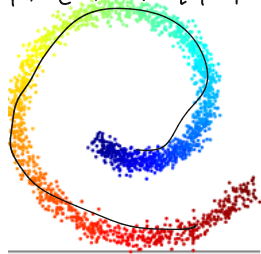


- produce a k nearest neighbor graph
- connect points close together along spiral
- find Y, Z s.t. $A \approx YZ^T$



SPECTRAL EMBEDDING

(x_1, x_2)
 (x_1, x_2, x_1^2, x_2^2)



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

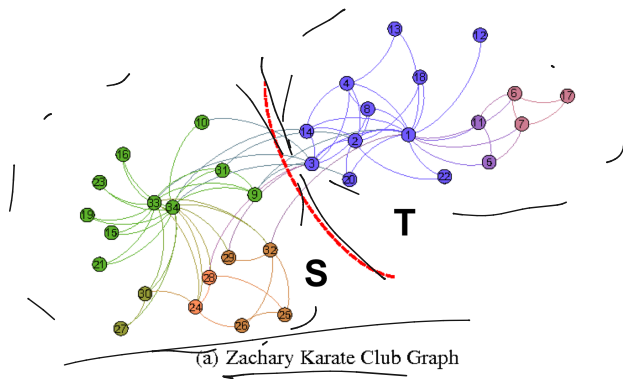
Kernel methods → kernel PCA
random walks on graphs
Feature transformations
neural networks

DeepWalk
node2Vec

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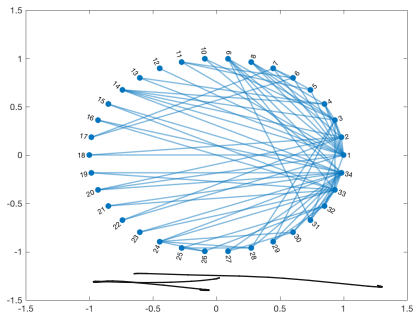
Community detection in naturally occurring networks.



SPECTRAL CLUSTERING

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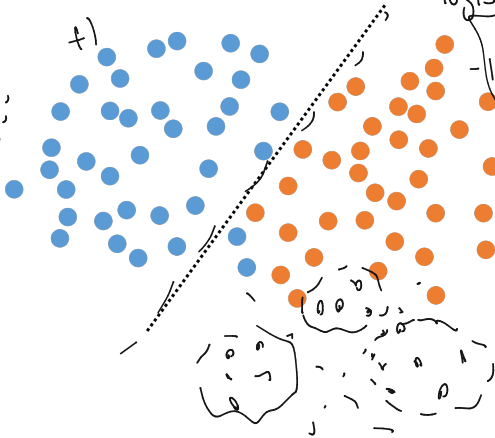
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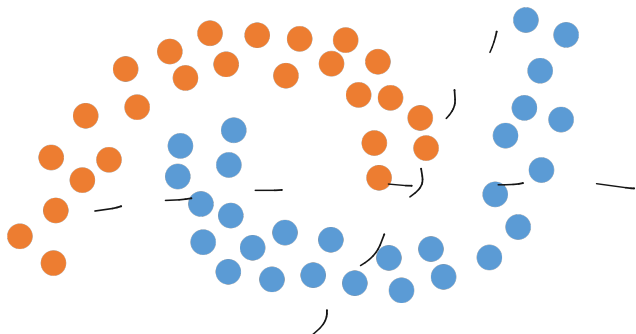
Linearly separable data.



SVM
Perceptron
logistic regression
decision trees
↳ do non-linear separation
k-mean clustering

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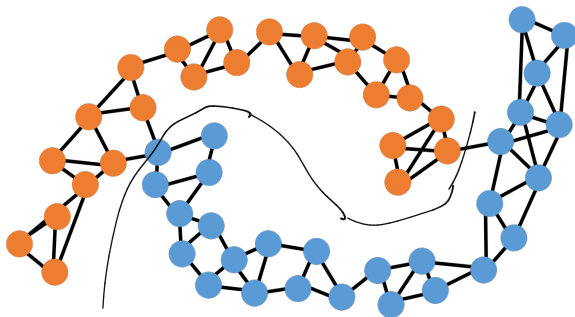
Non-linearly separable data k -nearest neighbor graph.



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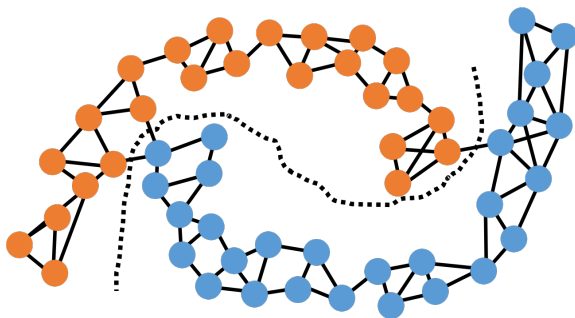
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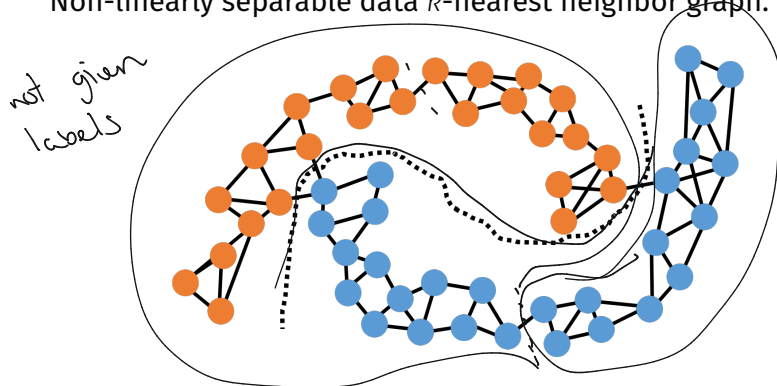
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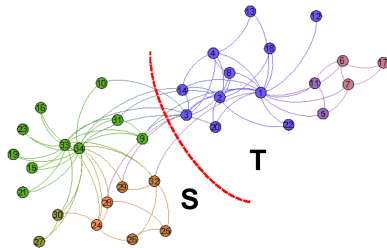
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Non-linearly separable data k -nearest neighbor graph.



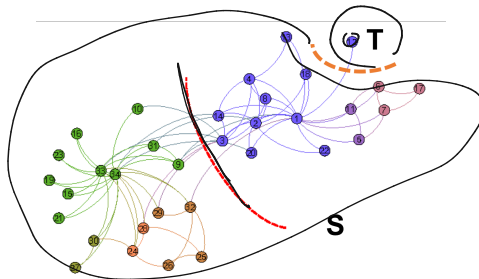
This Class: Find this cut using eigendecomposition. First – motivate why this type of approach makes sense.

Simple Idea: Partition clusters along minimum cut in graph.



(a) Zachary Karate Club Graph

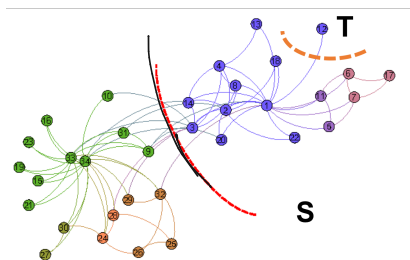
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Small cuts are often not informative.

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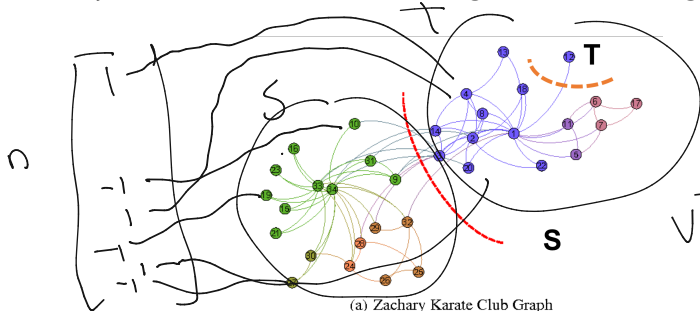
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Solution: Encourage cuts that separate large sections of the graph.

CUT MINIMIZATION

(dense subgraph mining)

Simple Idea: Partition clusters along minimum cut in graph.



(a) Zachary Karate Club Graph

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

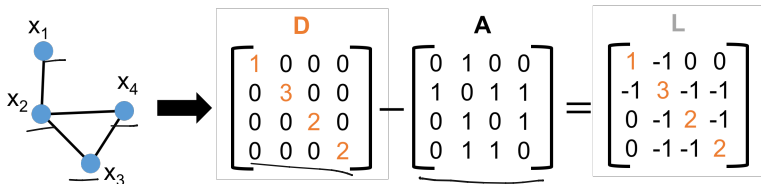
Small cuts are often not informative.

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

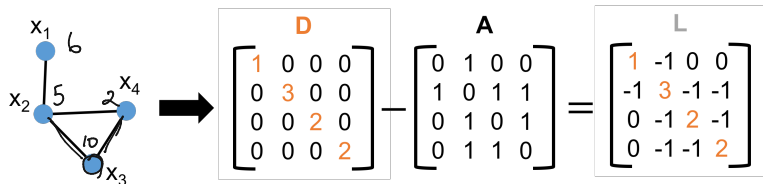
For a graph with adjacency matrix A and degree matrix D, L = D - A is the **graph Laplacian**.



THE LAPLACIAN VIEW

$$\begin{bmatrix} 6 & 5 & 10 & 2 \end{bmatrix}^T \begin{bmatrix} L \end{bmatrix} \begin{bmatrix} 6 \\ 5 \\ 10 \\ 2 \end{bmatrix} = \sum_{i,j \in E} (v_i - v_j)^2$$

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



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

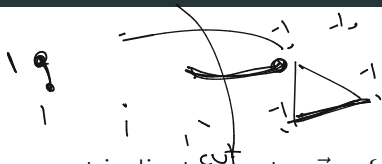
$$\vec{v} = \begin{bmatrix} 6 \\ 5 \\ 10 \\ 2 \end{bmatrix}$$

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

$$(6-5)^2 + (5-2)^2 + (5-10)^2 + (10-2)^2$$

Exercise: prove this.

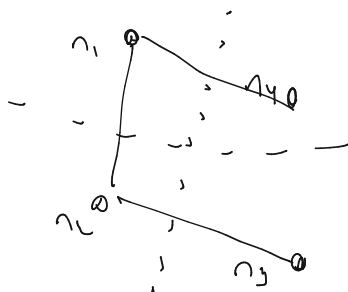
THE LAPLACIAN VIEW



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 $i \in T$:

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

$$\vec{v}_1 \quad \begin{bmatrix} 1 \\ 1 \\ -1 \\ -1 \end{bmatrix} \quad \vec{v}_2 \quad \begin{bmatrix} -1 \\ -1 \\ 1 \\ -1 \end{bmatrix}$$



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

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