Machine Learning for Data Science (CS4786)
Lecture 10

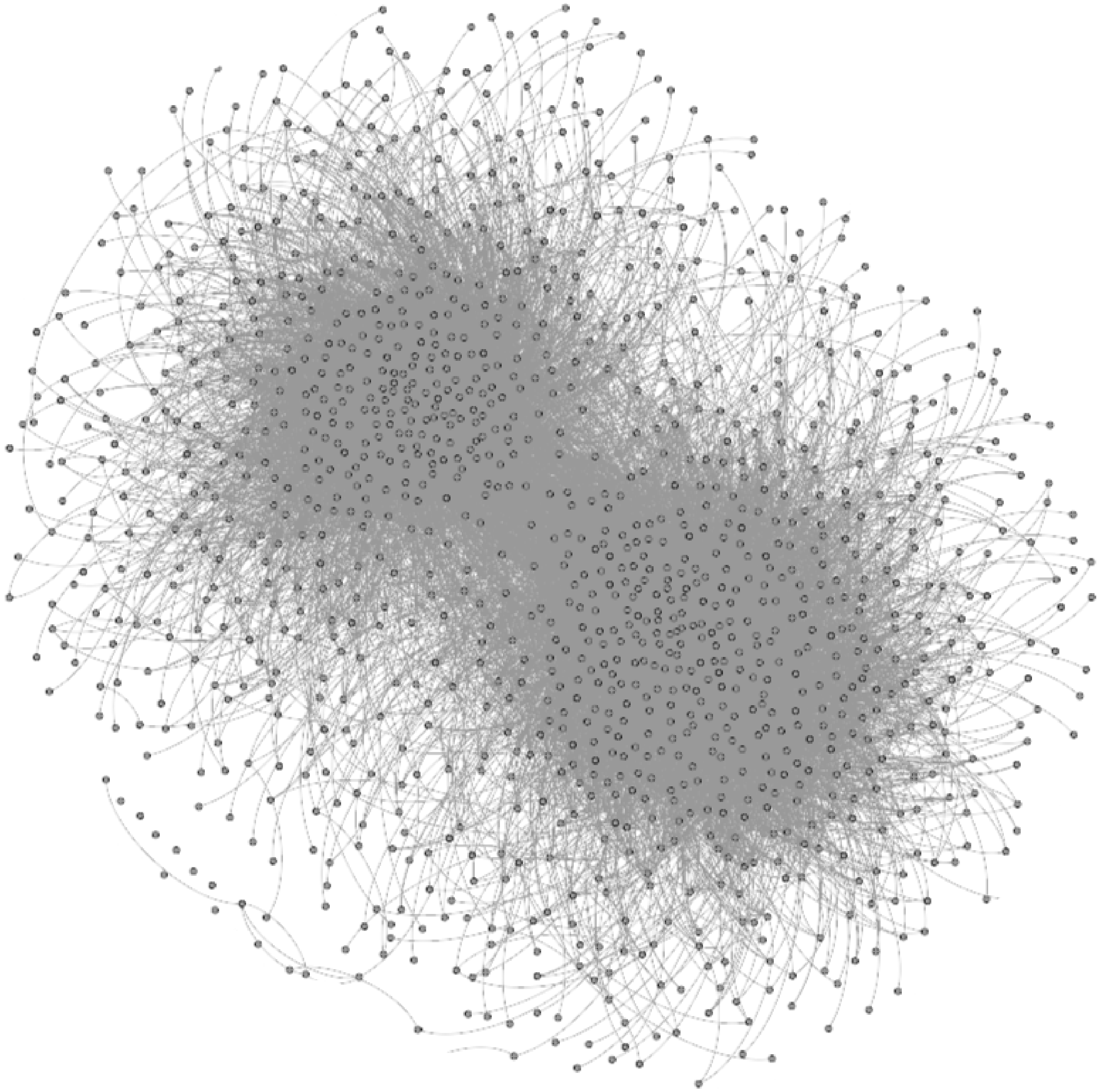
Spectral Clustering

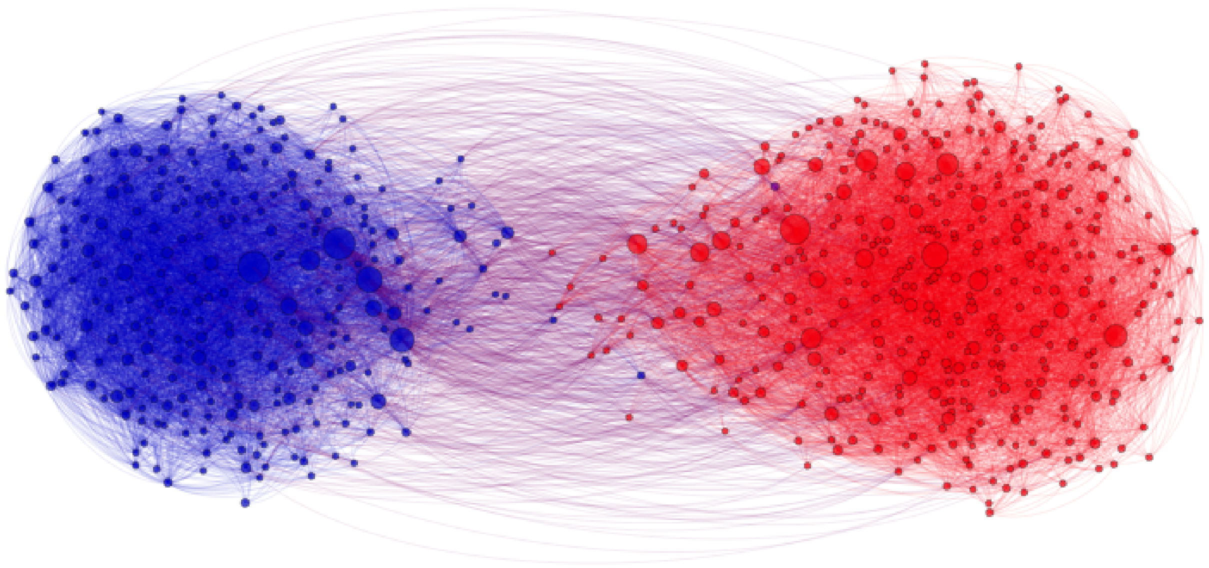
Course Webpage :
http://www.cs.cornell.edu/Courses/cs4786/2016fa/

Survey

- There will be 2 surveys and the final course eval
  - If overall class participation is above 90% on all 3 I will drop all your worst assignments
- Survey one posted on CMS due by 28th sep
- Surveys are all completely anonymous and will help me make the class more fun. So be open.

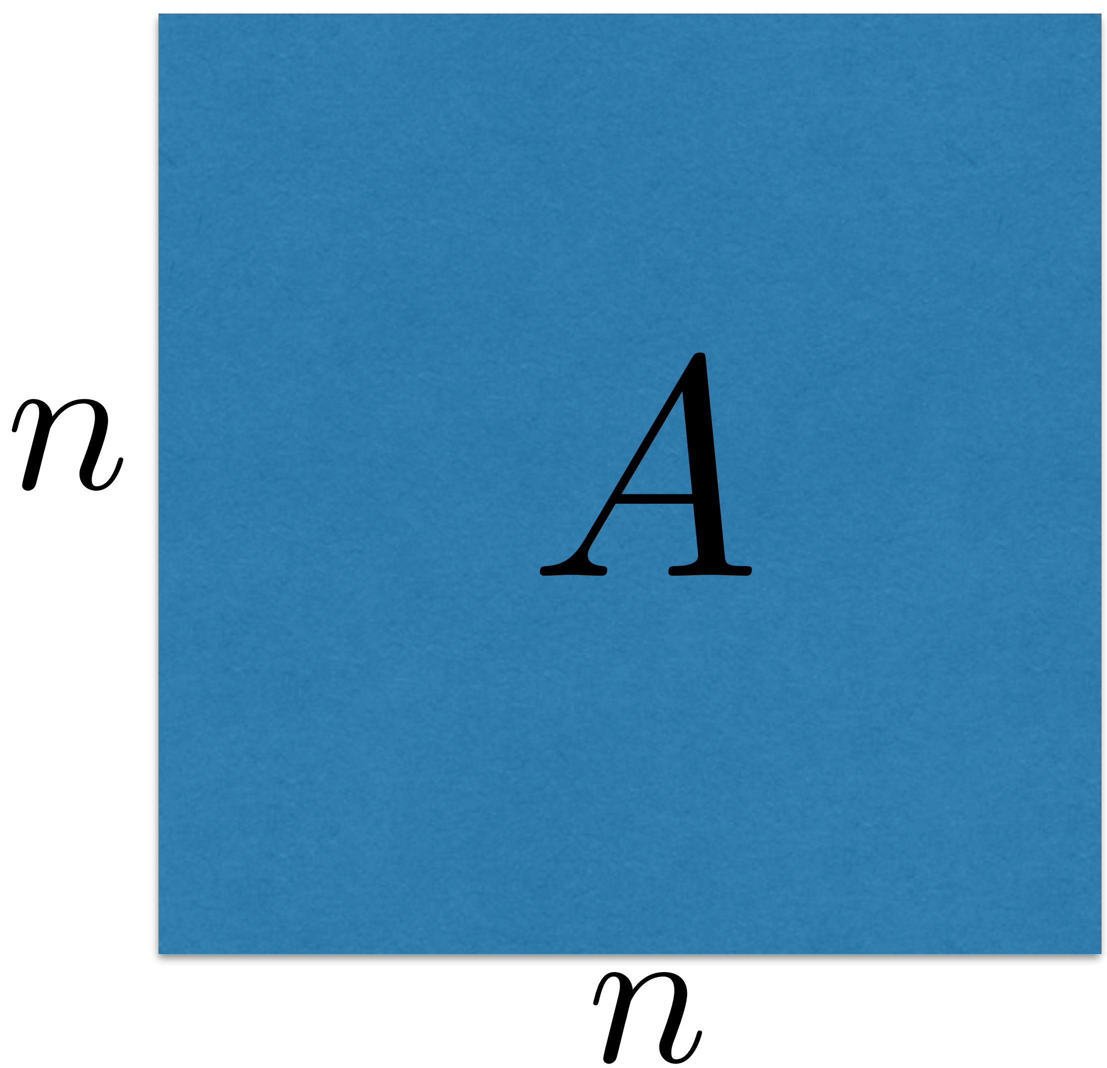
Spectral Clustering





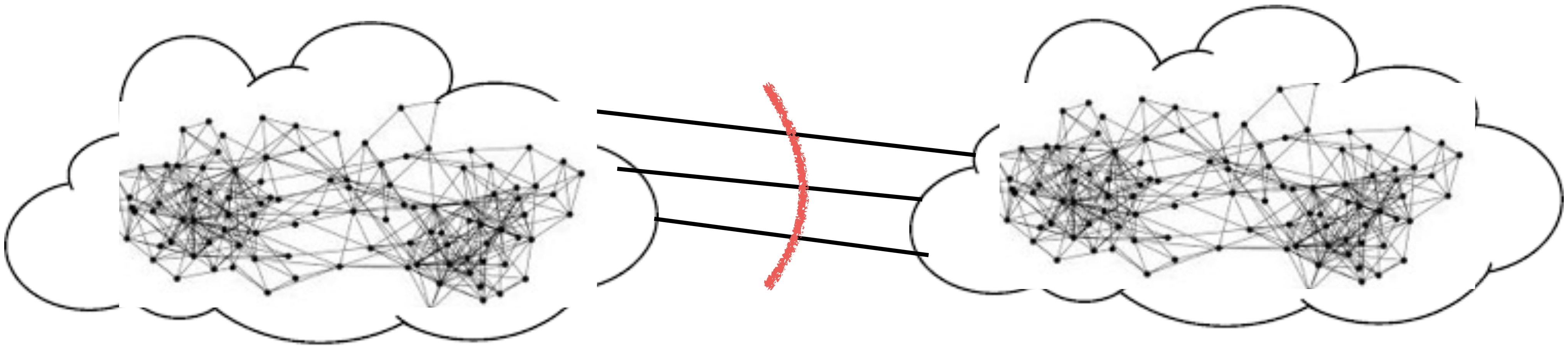
- Cluster nodes in a graph.
- Analysis of social network data.

$$A_{i,j} = \begin{cases} 1 & \text{if } (i,j) \in E \\ 0 & \text{otherwise} \end{cases}$$



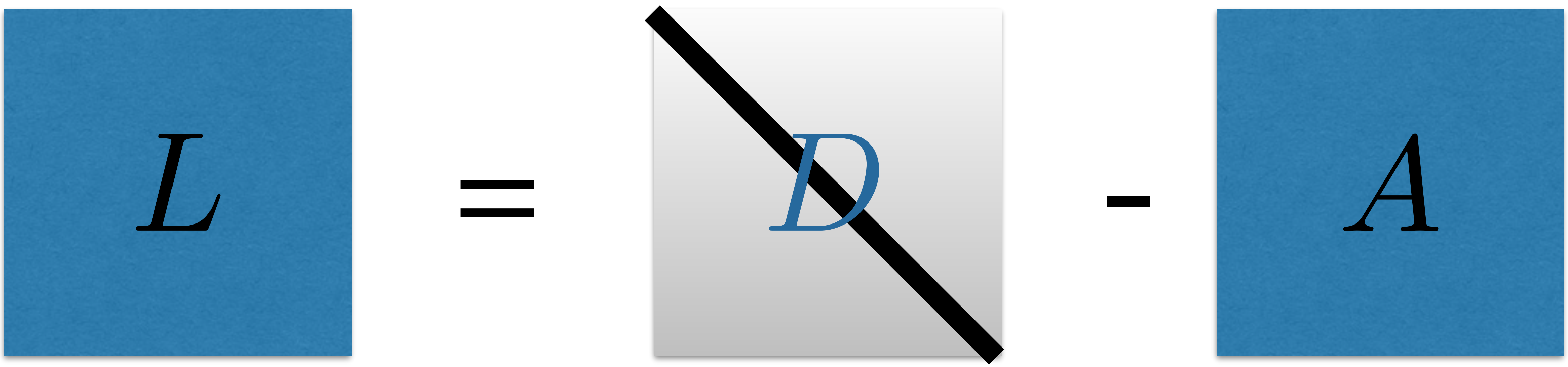
A is adjacency matrix of a graph

Example



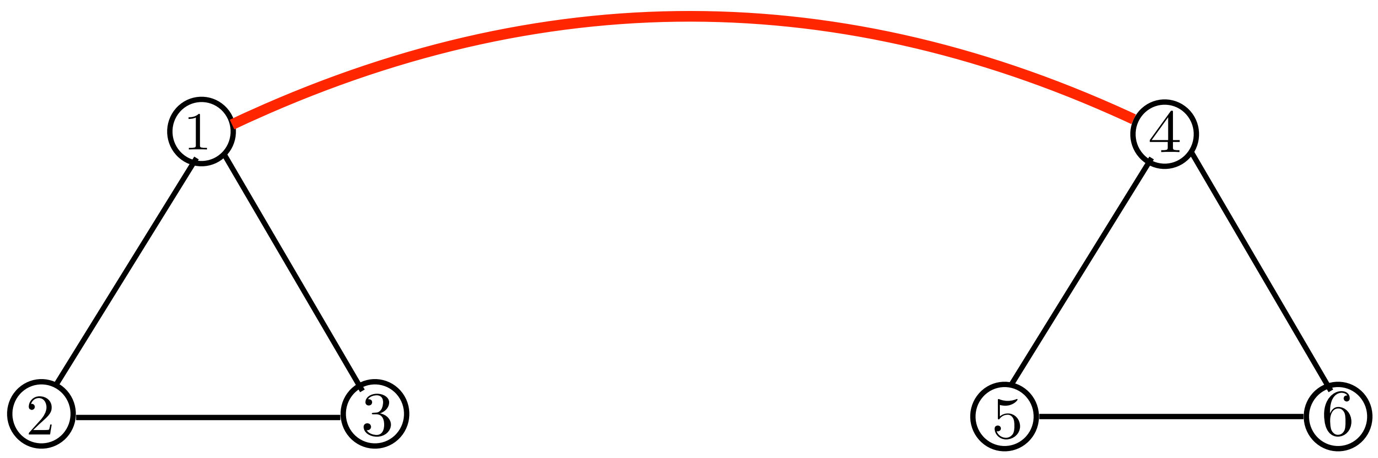
Cut as few edges as possible

Spectral Clustering



$$D_{i,i} = \sum_{j=1}^{n} A_{i,j}$$

EXAMPLE



Graph Clustering: Cuts

- Partition nodes so that as few edges are cut (Mincut)
- What has this got to do with the Laplacian matrix?

CUTS AND LAPLACIAN

Consider case when we have/want 2 clusters. Let $c_j = -1$ if x_j belongs to cluster 0 and $c_j = 1$ if x_j belongs to cluster 1

$$\text{CUT} = \sum_{(i,j)\in E} \mathbf{1}_{c_i \neq c_j} = \frac{1}{2} c^\top L c$$

Cuts and Laplacian

$$\mathrm{Cut}(c) = \sum_{(i,j)\in E} \mathbf{1}_{c_i \neq c_j} = \sum_{i=1}^{n}\sum_{j=1}^{n} A_{i,j}\mathbf{1}_{c_i\neq c_j}$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n} A_{i,j}\frac{1}{4}(c_i - c_j)^2$$

$$= \sum_{i=1}^{n}\sum_{j=1}^{n} A_{i,j}\frac{1}{4}(c_i^2 + c_j^2 - 2c_ic_j)$$

$$= \frac{1}{4}\left(\sum_{i=1}^{n}\left(\sum_{j=1}^{n} A_{i,j}\right)c_i^2 + \sum_{j=1}^{n}\left(\sum_{i=1}^{n} A_{i,j}\right)c_j^2 - 2\sum_{i=1}^{n}\sum_{j=1}^{n} A_{i,j}c_ic_j)\right)$$

$$= \frac{1}{4}\left(2\sum_{i=1}^{n} D_{i,i}c_i^2 - 2\sum_{i=1}^{n}\sum_{j=1}^{n} A_{i,j}c_ic_j)\right)$$

$$= \frac{1}{2}\left(c^\top Dc - c^\top Ac\right) = \frac{1}{2}c^\top Lc$$

Spectral Clustering, K = 2

Hence to find the solution we need to solve for

$$\text{Minimize } c^\top L c \quad \text{s.t. } \forall i \in [n], |c_i| = 1$$

Since $\forall i \in [n], |c_i| = 1$, we have $\|c\|_2 = \sqrt{n}$ and so relaxing (approximating) the optimization:

$$\text{Minimize } c^\top L c \quad \text{s.t. } \|c\|_2 = \sqrt{n}$$

Hence solution c to above is an Eigen vector, first smallest one is the all 1's vector (for connected graph), second smallest one is our solution

To get clustering assignment we simply threshold at 0

Spectral Clustering, $K > 2$

- Solution obtained by considering the second smallest up to K^{th} smallest eigenvectors
- If instead of $c_i = \pm 1$ make for each $k \in [K]$, c_i^k to be indicator of whether point i belongs to cluster K or not, then

$$\text{Cut} = \sum_{k=1}^{K} (c^k)^\top L c^k$$

Spectral Clustering Algorithm (Unnormalized)

1. Given matrix A calculate diagonal matrix D s.t. $D_{i,i} = \sum_{j=1}^{n} A_{i,j}$
2. Calculate the Laplacian matrix $L = D - A$
3. Find eigen vectors $\mathbf{v}_1, \ldots, \mathbf{v}_n$ of L (ascending order of eigenvalues)
4. Pick the K eigenvectors with smallest eigenvalues to get $\mathbf{y}_1, \ldots, \mathbf{y}_n \in \mathbb{R}^K$
5. Use K-means clustering algorithm on $\mathbf{y}_1, \ldots, \mathbf{y}_n$

$\mathbf{y}_1, \ldots, \mathbf{y}_n$ are called spectral embedding

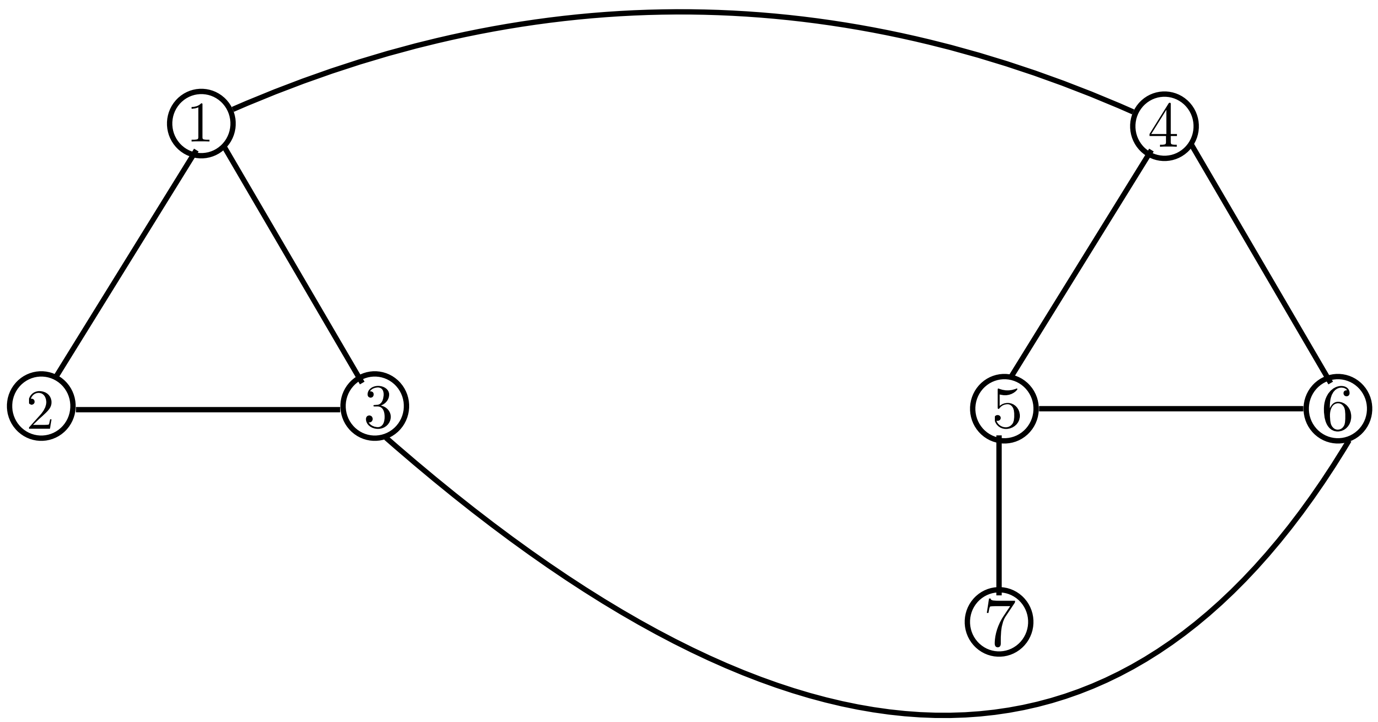
Embeds the n nodes into K-1 dimensional vectors

Spectral Clustering (Unnormalized)

- Min-cut on a graph can be efficiently computed
- Why bother with the approximate algorithm
- Is cut even a good measure?

Normalized Cut

- Why cut is perhaps not a good measure?



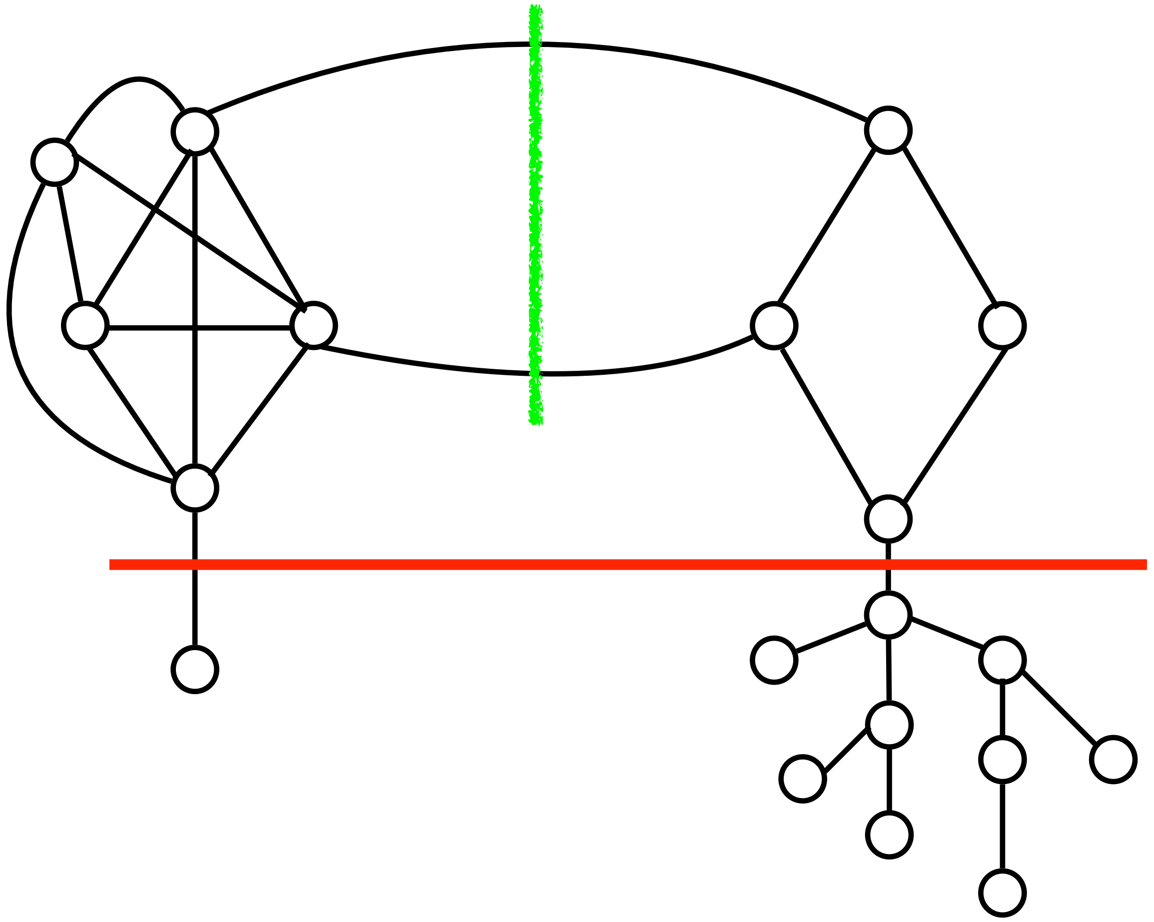
Ratio Cut

- Why cut is perhaps not a good measure?
- Fixes?

Ratio Cut

- Why cut is perhaps not a good measure?

- Fixes? Perhaps Ratio Cut : $\text{CUT}(C_1, C_2)\left(\frac{1}{|C_1|} + \frac{1}{|C_2|}\right)$

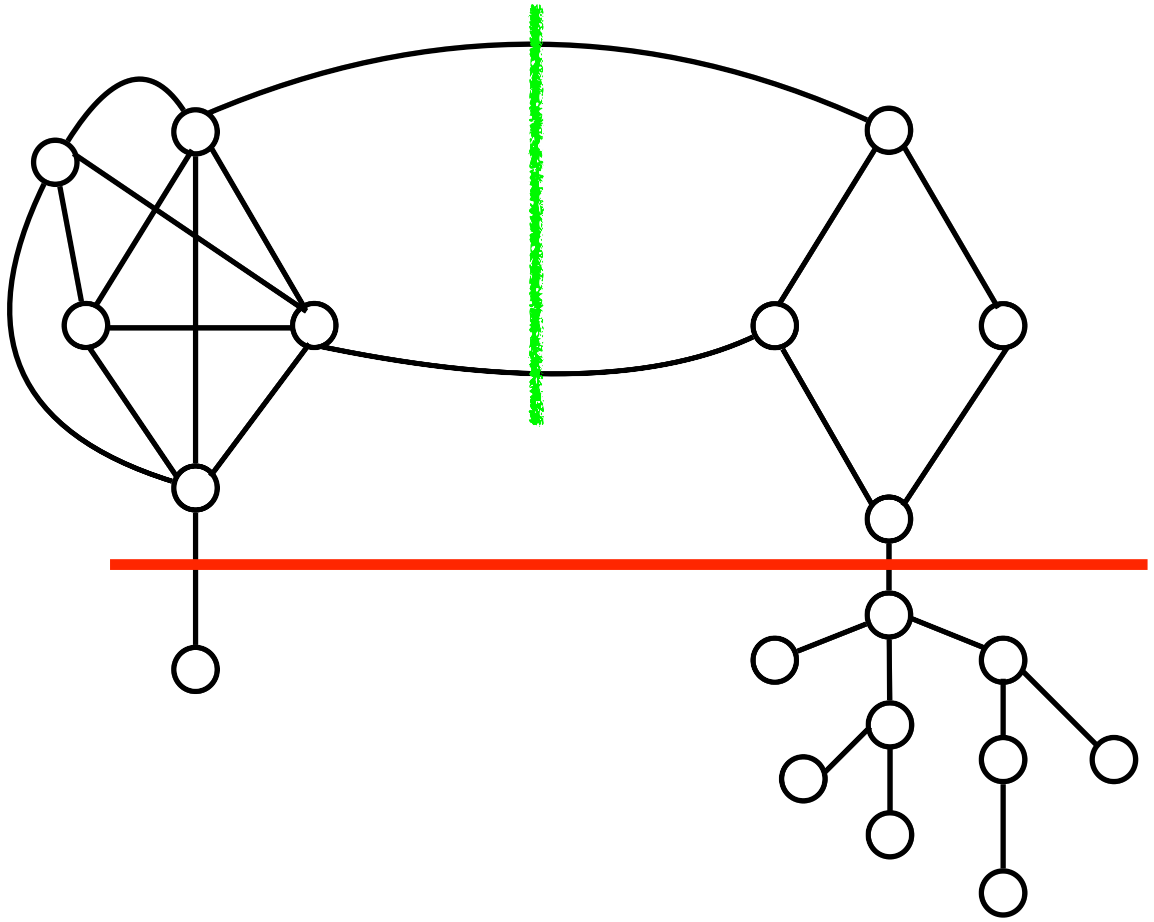


Normalized Cut

- Normalized cut: Minimize sum of ratio of number of edges cut per cluster and number of edges within cluster

$$\mathrm{NCUT} = \sum_j \frac{\mathrm{CUT}(C_j)}{\mathrm{Edges}(C_j)}$$

$$\mathrm{Edges}(C_i) = \mathrm{degree}(C_i) = \sum_{t \in C_i} D_{t,t}$$



Normalized Cut

- Normalized cut: Minimize sum of ratio of number of edges cut per cluster and number of edges within cluster

$$\text{NCUT} = \sum_j \frac{\text{CUT}(C_j)}{\text{Edges}(C_j)}$$

- Example $K = 2$

$$\text{Edges}(C_i) = \text{degree}(C_i) = \sum_{t \in C_i} D_{t,t}$$

$$\text{CUT}(C_1, C_2)\left(\frac{1}{\text{Edges}(C_1)} + \frac{1}{\text{Edges}(C_2)}\right)$$

- This is an NP hard problem! …so relax

Normalized Cut

- Set $c_i = \begin{cases} \sqrt{\frac{\text{Edges}(C_2)}{\text{Edges}(C_1)}} & \text{if } i \in C_1 \\ -\sqrt{\frac{\text{Edges}(C_1)}{\text{Edges}(C_2)}} & \text{otherwise} \end{cases}$
- Verify that $c^\top L c = |E| \times \text{NCut}$ and $c^\top D c = |E|$ (and $Dc \perp \mathbf{1}$)
- Hence we relax Minimize NCUT(C) to

$$\text{Minimize } \frac{c^\top L c}{c^\top D c} \qquad \text{s.t. } Dc \perp \mathbf{1}$$

- Solution: Find second smallest eigenvectors of $\tilde{L} = I - D^{-1/2} A D^{-1/2}$

SPECTRAL CLUSTERING ALGORITHM (NORMALIZED)

1. Given matrix A calculate diagonal matrix D s.t. $D_{i,i} = \sum_{j=1}^{n} A_{i,j}$
2. Calculate the normalized Laplacian matrix $\tilde{L} = I - D^{-1/2} A D^{-1/2}$
3. Find eigen vectors $\mathbf{v}_1, \ldots, \mathbf{v}_n$ of $\tilde{L}$ (ascending order of eigenvalues)
4. Pick the K eigenvectors with smallest eigenvalues to get $\mathbf{y}_1, \ldots, \mathbf{y}_n \in \mathbb{R}^K$
5. Use K-means clustering algorithm on $\mathbf{y}_1, \ldots, \mathbf{y}_n$

NORMALIZED CUT: ALTERNATE VIEW

- If we perform random walk on graph, its the partition of graph into group of vertices such that the probability of transiting from one group to another is minimized
- Transition matrix: $D^{-1}A$
- Largest eigenvalues and eigenvectors of above matrix correspond to smallest eigenvalues and eigenvectors of $D^{-1}L = I - D^{-1}A$
- For K-nearest neighbor graph (K-regular), same as normalized Laplacian