STA 221: LECTURE 6

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Spectral Clustering

Graph Clustering

- Given a graph $G = (V, E, W)$

  V: nodes $\{v_1, \cdots, v_n\}$

  E: edges $\{e_1, \cdots, e_m\}$

  W: weight matrix

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

- Goal: Partition V into k clusters of nodes

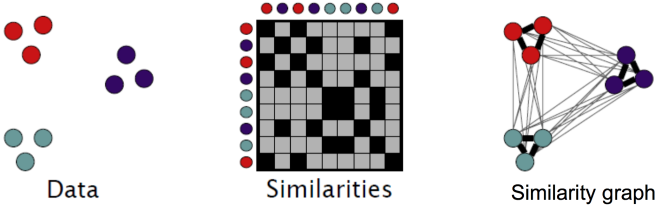
$$V = V_1 \cup V_2 \cup \cdots \cup V_k, \quad V_i \cap V_j = \phi, \ \forall i, j$$

Similarly Graph

- Example: similarity graph
- Given samples $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n$
- Weight (similarities) indicates "closeness of samples"

Similarity Graph: G(V,E,W)

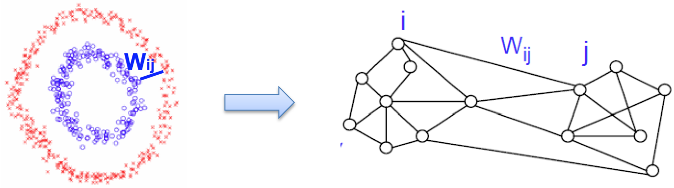
V – Vertices (Data points)
E – Edge if similarity > 0
W - Edge weights (similarities)



Partition the graph so that edges within a group have large weights and edges across groups have small weights.

Similarity Graph

E.g., Gaussian kernel $W_{ij} = e^{-\|\boldsymbol{x}_i - \boldsymbol{x}_j\|^2/\sigma^2}$

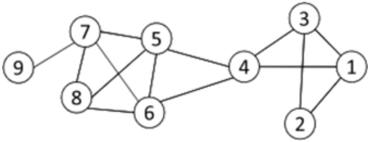


Data clustering

$G = \{V,E\}$

- Nodes: users in social network
- Edges: $W_{ij} = 1$ if user i and j are friends,
  otherwise $W_{ij} = 0$

Graph Representation



Matrix Representation

Node	1	2	3	4	5	6	7	8	9
1	-	1	1	1	0	0	0	0	0
2	1	-	1	0	0	0	0	0	0
3	1	1	-	1	0	0	0	0	0
4	1	0	1	-	1	1	0	0	0
5	0	0	0	1	-	1	1	1	0
6	0	0	0	1	1	-	1	1	0
7	0	0	0	0	1	1	-	1	1
8	0	0	0	0	1	1	1	-	0
9	0	0	0	0	0	0	1	0	-

Partitioning into Two Clusters

- Partition graph into two sets V_1, V_2 to minimize the cut value:

$$cut(V_1, V_2) = \sum_{v_i \in V_1, v_j \in V_2} W_{ij}$$

- Also, the size of V_1, V_2 needs to be similar (balance)
- One classical way of enforcing balance:

$$\min_{V_1, V_2} \ \text{cut}(V_1, V_2)$$
$$\text{s.t.} \ |V_1| = |V_2|, \quad V_1 \cup V_2 = \{1, \cdots, n\}, V_1 \cap V_2 = \phi$$

$\Rightarrow$ this is NP-hard (cannot be solved in polynomial time, a.k.a. "bad problems")

Kernighan-Lin Algorithm

- Starts with some partitioning V_1, V_2
- Calculate change in cut if 2 vertices are swapped
- Swap the vertices (1 in V_1 & 1 in V_2) that decease the cut the most
- Iterative until convergence
- Used when we need exact balanced clusters

  (e.g., circuit design)

Objective function that considers balance

- Ratio-Cut:

$$\min_{V_1, V_2} \left\{ \frac{\mathrm{Cut}(V_1, V_2)}{|V_1|} + \frac{\mathrm{Cut}(V_1, V_2)}{|V_2|} \right\} := \mathrm{RC}(V_1, V_2)$$

- Normalized-Cut:

$$\min_{V_1, V_2} \left\{ \frac{\mathrm{Cut}(V_1, V_2)}{\deg(V_1)} + \frac{\mathrm{Cut}(V_1, V_2)}{\deg(V_2)} \right\} := \mathrm{NC}(V_1, V_2),$$

where

$$\deg(V_c) := \sum_{v_i \in V_c, (i,j) \in E} W_{i,j} = \mathrm{links}(V_c, V)$$

Generalize to k clusters

- Ratio-Cut:

$$\min_{V_1,\cdots,V_k} \sum_{c=1}^{k} \frac{\mathrm{Cut}(V_c, V - V_c)}{|V_c|}$$

- Normalized-Cut:

$$\min_{V_1,\cdots,V_k} \sum_{c=1}^{k} \frac{\mathrm{Cut}(V_c, V - V_c)}{\deg(V_c)}$$

- Recall $\deg(V_c) = \text{links}(V_c, V)$
- Define a diagonal matrix

$$D = \begin{bmatrix} \deg(V_1) & 0 & 0 & \cdots \\ 0 & \deg(V_2) & 0 & \cdots \\ 0 & 0 & \deg(V_3) & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

- $\mathbf{y}_c = \{0, 1\}^n$: indicator vector for the c-th cluster
- We have

$$\mathbf{y}_c^T \mathbf{y}_c = |V_c|$$
$$\mathbf{y}_c^T D \mathbf{y}_c = \deg(V_c)$$
$$\mathbf{y}_c^T W \mathbf{y}_c = \text{links}(V_c, V_c)$$

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$$\begin{aligned} \mathbf{y}_c^T \mathbf{y}_c &= |V_c| \\ \mathbf{y}_c^T D \mathbf{y}_c &= \deg(V_c) \\ \mathbf{y}_c^T W \mathbf{y}_c &= \text{links}(V_c, V_c) \end{aligned}$$

Ratio Cut

- Rewrite the ratio-cut objective:

$$
\begin{aligned}
RC(V_1, \cdots, V_k) &= \sum_{c=1}^{k} \frac{\mathrm{Cut}(V_c, V - V_c)}{|V_c|} \\
&= \sum_{c=1}^{k} \frac{\deg(V_c) - \mathrm{links}(V_c, V_c)}{|V_c|} \\
&= \sum_{c=1}^{k} \frac{\mathbf{y}_c^T D \mathbf{y}_c - \mathbf{y}_c^T W \mathbf{y}_c}{\mathbf{y}_c^T \mathbf{y}_c} \\
&= \sum_{c=1}^{k} \frac{\mathbf{y}_c^T (D - W) \mathbf{y}_c}{\mathbf{y}_c^T \mathbf{y}_c} \\
&= \sum_{c=1}^{k} \frac{\mathbf{y}_c^T L \mathbf{y}_c}{\mathbf{y}_c^T \mathbf{y}_c} \quad (L = D - W \text{ is “Graph Laplacian”})
\end{aligned}
$$

More on Graph Laplacian

- L is symmetric positive semi-definite
- For any $\boldsymbol{x}$,

$$\boldsymbol{x}^T L \boldsymbol{x} = \frac{1}{2} \sum_{(i,j)} W_{ij}(x_i - x_j)^2$$

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- ▷ For any $\boldsymbol{x}$,

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- We have shown Ratio-Cut is equivalent to

$$\text{RCut} = \sum_{c=1}^{k} \frac{\mathbf{y}_c^T L \mathbf{y}_c}{\mathbf{y}_c^T \mathbf{y}_c} = \sum_{c=1}^{k} \left(\frac{\mathbf{y}_c}{\|\mathbf{y}_c\|}\right)^T L \frac{\mathbf{y}_c}{\|\mathbf{y}_c\|}$$

- Define $\bar{\mathbf{y}}_c = \mathbf{y}_c / \|\mathbf{y}_c\|$ (normalized indicator),

$$Y = [\bar{\mathbf{y}}_1, \bar{\mathbf{y}}_2, \cdots, \bar{\mathbf{y}}_k] \; \Rightarrow \; Y^T Y = I$$

- Relaxed to real valued problem:

$$\min_{Y^T Y = I} \text{Trace}(Y^T L Y)$$

- Solution: Eigenvectors corresponding to the smallest k eigenvalues of L

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Solving Ratio-Cut

- ▷ We have shown Ratio-Cut is equivalent to

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- ▷ Let $Y^* \in \mathbb{R}^{n \times k}$ be these eigenvectors. Are we done?
- ▷ No, Y^* does not have 0/1 values (not indicators)
  (since we are solving a **relaxed** problem)
- ▷ Solution: Run k-means on the rows of Y^*
- ▷ Summary of Spectral clustering algorithms:
  - Compute $Y^* \in \mathbb{R}^{n \times k}$: eigenvectors corresponds to k smallest eigenvalues of (normalized) Laplacian matrix
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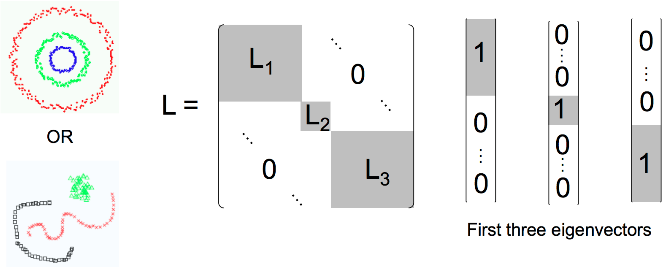
- If graph is disconnected (k connected components), Laplacian is block diagonal and first k eigen-vectors are:



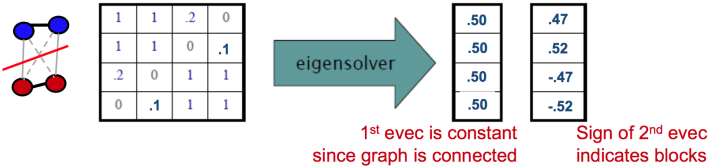
Eigenvectors of Laplacian

- What if the graph is connected?
- There will be only one smallest eigenvalue/eigenvector:

$$L\mathbf{1} = (D - A)\mathbf{1} = 0$$

($\mathbf{1} = [1, 1, \cdots, 1]^T$ is the eigenvector with eigenvalue 0)

- However, the 2nd to k-th smallest eigenvectors are still useful for clustering



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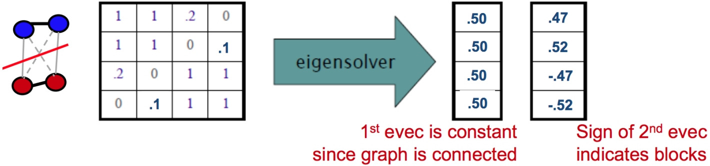

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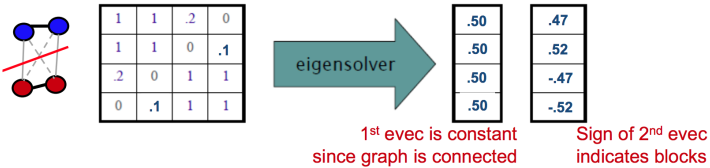

Normalized Cut

- Rewrite Normalized Cut:

$$\text{NCut} = \sum_{c=1}^{k} \frac{\text{Cut}(V_c, V - V_c)}{\text{deg}(V_c)}$$

$$= \sum_{c=1}^{k} \frac{\mathbf{y}_c^T (D - A)\mathbf{y}_c}{\mathbf{y}_c^T D \mathbf{y}_c}$$

- Let $\tilde{\mathbf{y}}_c = \frac{D^{1/2}\mathbf{y}_c}{\|D^{1/2}\mathbf{y}_c\|}$, then

$$\text{NCut} = \sum_{c=1}^{k} \frac{\tilde{\mathbf{y}}_c^T D^{-1/2}(D - A)D^{-1/2}\tilde{\mathbf{y}}_c}{\tilde{\mathbf{y}}_c^T \tilde{\mathbf{y}}_c}$$

- Normalized Laplacian:

$$\tilde{L} = D^{-1/2}(D - A)D^{-1/2} = I - D^{-1/2}AD^{-1/2}$$

- Normalized Cut $\rightarrow$ eigenvectors correspond to the smallest eigenvalues of $\tilde{L}$

- Kmeans: decision boundary is linear
- Spectral clustering: boundary can be non-convex curves

  σ in $W_{ij} = e^{\frac{-\|\mathbf{x}_i - \mathbf{x}_j\|^2}{\sigma^2}}$ controls the clustering results (focus on local or global structure)

Kmeans vs Spectral Clustering