Clustering

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1 Clustering of a Graph and Eigenvalue

Informally, "clustering" is grouping vertices such that there are more connectivity inside each group compare to between groups.

1.1 Conductance

Definition 1.1. Volume: let $S \subseteq V$, $\operatorname{vol}(S) \stackrel{\text{def}}{=} \sum_{v \in S} d_v$ where $d_v = \deg(v) = \mathbf{D}_{v,v}$

Lemma 1.2. Define the indicator of set S as

$$\mathbf{1}_{S}(v) = \begin{cases} 1, & v \in S \\ 0, & otherwise \end{cases}$$

Then

$$\mathbf{1}_S^T \mathbf{D} \mathbf{1}_S = \mathsf{vol}(S)$$

Definition 1.3. Define Boundary of S as

$$E(S,\overline{S}) = \{(u,v) | (u,v) \in E, u \in S, v \in V \setminus S\},\$$

where \overline{S} is the complement set.

Definition 1.4. Define conductance of S measured in graph G to be

$$\phi_G(S) \stackrel{\text{def}}{=} \frac{|E(S,\overline{S})|}{\min\{\operatorname{vol}(S),\operatorname{vol}(V \setminus S)\}}$$

and define conductance of graph G to be

$$\phi(G) \stackrel{\text{def}}{=} \min_{\substack{S \subseteq V \\ S \neq \emptyset, V}} \phi_G(S).$$

Computing $\phi(G)$ is called "minimum conductance problem", and it is famously NP hard. However, we can connect conductance and eigenvalues.

1.2 Normalized Laplacian Matrix

Let $\nu_2 = \min_{y^\top \mathbf{D} \mathbf{1} = 0} \left(\frac{y^\top \mathbf{L} y}{y^\top \mathbf{D} y} \right).$

Define $x = \mathbf{D}^{\frac{1}{2}} y$ (note $\mathbf{D}^{\frac{1}{2}}$ is replacing each of the diagonal entries in diagonal matrix \mathbf{D} with square root), we can write $y^{\top}\mathbf{D}y = x^{\top}x$.

Note we are assuming the graph G is connected, then diagonal of D is strictly non-negative, so the mapping between x and y is a bijection, which gives us $x = \mathbf{D}^{\frac{1}{2}}y \Leftrightarrow y = \mathbf{D}^{-\frac{1}{2}}x \Rightarrow y^{\top}\mathbf{D}y = x^{\top}x$. Then we can rewrite ν_2 as

$$\nu_2 = \min_{x^\top \left(\mathbf{D}^{\frac{1}{2}}\mathbf{1}\right) = 0} \frac{x^\top \mathbf{D}^{-\frac{1}{2}} \mathbf{L} \mathbf{D}^{-\frac{1}{2}} x}{x^\top x}.$$

Definition 1.5. Define Normalized Laplacian Matrix as

$$\mathbf{N} \stackrel{\text{def}}{=} \mathbf{D}^{-\frac{1}{2}} \mathbf{L} \mathbf{D}^{-\frac{1}{2}}$$

We also claim that:

$$\begin{aligned} \lambda_1(\mathbf{N}) &= 0\\ \psi_1 &= \mathbf{D}^{\frac{1}{2}} \mathbf{1}\\ \nu_2 &= \min_{x^\top \psi_1 = 0} \frac{x^\top \mathbf{N} x}{x^\top x}\\ &= \lambda_2(\mathbf{N}) \end{aligned}$$

1.3 Cheeger's Inequality

Theorem 1.6.

$$\frac{\nu_2}{2} \le \phi(G) \le \sqrt{2\nu_2}, \nu_2 \le 2$$

For example, if $\nu_2 = 0.01 \Rightarrow 0.005 \le \phi(G) \le 0.14$ We'll first prove the left hand side, $\frac{\nu_2}{2} \le \phi(G)$.

Proof. By definition, we know $\exists S \ s.t. \ \phi(G) = \phi_G(S) = \frac{|E(S,\overline{S})|}{\operatorname{vol}(S)}$ and $\operatorname{vol}(S) \leq \operatorname{vol}(\overline{S})$. Recall $\nu_2 = \min_{y^\top \mathbf{D1} = 0} \left(\frac{y^\top \mathbf{L}y}{y^\top \mathbf{D}y} \right)$ and $\mathbf{1}_S^\top \mathbf{D1}_S = \operatorname{vol}(S)$, we have

$$\mathbf{1}_{S}^{\top}\mathbf{L}\mathbf{1}_{S} = \sum_{(u,v)\in E} \left(\mathbf{1}_{S}(u) - \mathbf{1}_{S}(v)\right)^{2}$$

note

$$\left(\mathbf{1}_{S}(u) - \mathbf{1}_{S}(v)\right)^{2} = \begin{cases} 1, & \mathbf{1}_{S}(v) \neq \mathbf{1}_{S}(v) \Leftrightarrow (u, v) \in E(S, \overline{S}) \\ 0, & \text{otherwise} \end{cases}$$

therefore

$$\mathbf{1}_{S}^{\top}\mathbf{L}\mathbf{1}_{S} = \sum_{(u,v)\in E}\mathbf{1}[(u,v)\in E(S,\overline{S})] = |E(S,\overline{S})|$$

If we set $y = \mathbf{1}_S$, it would minimize $\frac{y^{\top} \mathbf{L} y}{y^{\top} \mathbf{D} y}$, however it may not satisfy $y^{\top} \mathbf{D} \mathbf{1} = 0$. In order to make y satisfy $y^{\top} \mathbf{D} \mathbf{1} = 0$, let $y = \mathbf{1}_S + c\mathbf{1}$, note we still have $y^{\top} \mathbf{L} y = |E(S, \overline{S})|$.

$$y^{\top} \mathbf{D} \mathbf{1} = 0 \Leftrightarrow c = \frac{-\mathbf{1}_{S}^{\top} \mathbf{D} \mathbf{1}}{\mathbf{1}^{\top} \mathbf{D} \mathbf{1}} = -\frac{\mathsf{vol}(S)}{\mathsf{vol}(V)}$$
(by previous lemma)

$$\begin{split} y^{\top} \mathbf{D} y &= \mathbf{1}_{S}^{\top} \mathbf{D} \mathbf{1}_{S} + 2c \mathbf{1}_{S}^{\top} \mathbf{D} \mathbf{1} + c^{2} \mathbf{1}^{\top} \mathbf{D} \mathbf{1} \\ &= \mathbf{1}_{S}^{\top} \mathbf{D} \mathbf{1}_{S} - \frac{\left(\mathbf{1}_{S}^{\top} \mathbf{D} \mathbf{1}\right)^{2}}{\mathbf{1}^{\top} \mathbf{D} \mathbf{1}} \\ &= \operatorname{vol}(S) - \frac{\operatorname{vol}(S)^{2}}{\operatorname{vol}(V)} \\ &= \operatorname{vol}(S) \left(1 - \frac{\operatorname{vol}(S)}{\operatorname{vol}(V)}\right) \\ &\geq \frac{\operatorname{vol}(S)}{2} \qquad (\text{since } \operatorname{vol}(S) \leq \operatorname{vol}(\overline{S})) \end{split}$$

Therefore

$$\frac{y^{\top} \mathbf{L} y}{y^{\top} \mathbf{D} y} = \frac{|E(S, \overline{S})|}{y^{\top} \mathbf{D} y} \\
\leq \frac{2|E(S, \overline{S})|}{\operatorname{vol}(S)} \\
= 2\phi_G(S) \\
= 2\phi(G) \qquad \text{(by assumption)} \\
\Rightarrow \nu_2 = \min_{y^{\top} \mathbf{D} \mathbf{1} = 0} \frac{y^{\top} \mathbf{L} y}{y^{\top} \mathbf{D} y} \leq 2\phi(G) \\
\Rightarrow \frac{\nu_2}{2} \leq \phi(G)$$

Lemma 1.7. Given y s.t. $y^{\top} \mathbf{D1} = 0$, we can find a distribution on t with $S_t \subseteq V$ s.t. $\operatorname{vol}(S_t) \leq \frac{\operatorname{vol}(V)}{2}$, and

$$\frac{\mathbb{E}_t |E(S_t, \overline{S_t})|}{\mathbb{E}_t \operatorname{vol}(S_t)} \leq \sqrt{\frac{2y^\top \mathbf{L} y}{y^\top \mathbf{D} y}}$$

Let t be independent choices, P_t be distribution of t, X_t , Y_t are variables depend on t with $Y_t \ge 0$.

We can prove that $\exists t \text{ s.t.}$

$$\frac{X_t}{Y_t} \le \frac{\mathbb{E}_t X_t}{\mathbb{E}_t Y_t} = \frac{\sum_t P_t X_t}{\sum_t P_t Y_t}$$

The proof is left as exercise. This implies that $\exists t, s.t.$

$$\frac{|E(S_t, \overline{S_t})|}{\operatorname{vol}(S_t)} \leq \sqrt{\frac{2y^\top \mathbf{L} y}{y^\top \mathbf{D} y}}$$

Furthermore, if y was the minimizing vector for ν_2 , then

$$\phi_S(S_t) = \frac{|E(S_t, \overline{S_t})|}{\operatorname{vol}(S_t)} \le \sqrt{2\nu_2}$$