k-way conductance to find k-clusters

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Abstract

Dividing a graph into k-clusters can be defined as dividing the vertex set into k mutually-disjoint subsets such that each induced subgraph is dense and sparsely connected to the rest of the original graph. For k=2, the conductance function helps us measure how good a 2-clustering is [7] [2] [6]. This paper defines and explores a novel k-way conductance function that will help us measure how good a k-clustering is.

1 Definitions and goals

Define \mathscr{S}_k as a k-way partition of V into non-empty, mutually disjoint subsets $\{S_i\}_{i=1}^k$:

$$\mathcal{S}_k = \{S_1, S_2, ..., S_k\}$$
 s.t.
$$S_i \subseteq V \text{ and } S_i \neq \emptyset \ \forall \ i$$

$$\bigcup_{i=1}^k S_i = V$$

$$S_i \bigcap S_j = \emptyset, \ \forall \ i \neq j$$

We define a novel k-way conductance function ψ over \mathscr{S}_k as follows:

$$\psi(\mathscr{S}_k) = \frac{1}{k} \cdot \frac{\sum_{i=1}^k cut(S_i)}{\min_{i=1}^k vol(S_i)}$$
(1)

Ideally, the goal would be to find a good k-clustering in the form of an optimal k-way partition \mathscr{S}_k^* :

$$\mathscr{S}_k^* = \operatorname{argmin}_{\mathscr{S}_k} \psi(\mathscr{S}_k)$$

It can be seen that for k = 2, the above problem is the minimum conductance problem.

Goals:

- Compare ψ with other existing k-way conductance functions. Present examples to compare k-clustering achieved by different k-way conductance functions.
- Analyse the complexity of the minimum k-way conductance problem.
- State and prove the bounds on the k-way conductance ψ (Cheeger's inequality equivalent).

2 Previous work

There have been other functions to measure how good a k-clustering is. One such measure is the following k-way conductance function [3]:

$$\phi(\mathscr{S}_k) = \max_{1 \le i \le k} \frac{cut(S_i)}{min\{vol(S_i), vol(\overline{S_i})\}}$$
 (2)

Once again, the goal would be to find a good k-clustering in the form of an optimal k-way partition \mathscr{S}_k^* :

$$\mathscr{S}_k^* = \operatorname{argmin}_{\mathscr{S}_k} \phi(\mathscr{S}_k)$$

i.e. we choose \mathscr{S}_k^* to minimize the conductance of the maximum conductance subset.

It can be seen that for k=2, once again, the above problem is the minimum conductance problem.

Similarities between ψ and ϕ : We can see that these two k-way conductance functions are very similar in the ways they are used. The goal in both cases is to find the k-way partition that minimizes these conductance functions. For k=2, both of them become equal to the usual conductance function.

3 Complexity analysis

Both k-way conductance functions ψ in (1), and ϕ in (2) become equal to the usual conductance function if we set k=2. And because minimizing conductance is an \mathcal{NP} -hard problem [8], minimizing k-way conductance ψ or ϕ is also an \mathcal{NP} -hard problem. Although, solutions to the decision version of both these k-way conductance problems are verifiable in polynomial time (to be precise, in O(|V|+|E|) time for either of them). Therefore, both these k-way conductance problems are \mathcal{NP} -complete.

4 k-way Cheeger's inequality

Let $\lambda_1 \leq \lambda_2 \leq ... \leq \lambda_{|V|}$ be the eigenvalues of the normalized laplacian matrix \mathcal{L} of graph G(V, E). Then:

Theorem 1. Cheeger's inequality [1] [3]

For a two-way partition $\{S, \overline{S}\}\$ on the graph G:

$$\frac{\lambda_2}{2} \le \frac{cut(S)}{min\{vol(S), vol(\overline{S})\}} \le \sqrt{2 \cdot \lambda_2}$$
 (3)

Theorem 2. Cheeger's inequality over k-way conductance ϕ [3] [5] [4]

For any k-way partition \mathcal{S}_k on the graph G:

$$\frac{\lambda_k}{2} \le \phi(\mathscr{S}_k) \le O(k^2) \sqrt{\lambda_k} \tag{4}$$

Theorem 3. Cheeger's inequality over k-way conductance ψ

For any k-way partition \mathcal{S}_k on the graph G:

$$\frac{\lambda_2}{k \cdot (k-1)} \le \psi(\mathscr{S}_k) \tag{5}$$

Theorem 3 defines only the lower-bound on the k-way conductance ψ . I could not complete the proof for an upper-bound. A novel proof of the lower bound in Theorem 3 is presented in the appendix.

As we can see, equations (4) and (5) are consistent with equation (3) if we set k=2.

5 Comparison with examples

We computed the optimal k-way partitions of some graphs based on the k-way conductance functions ψ and ϕ respectively. Since both these problems are hard, we use a brute force approach where we compute k-way conductance for all possible k-way partitions. The results are decent and similar for both approaches i.e. while minimizing ψ and ϕ respectively.

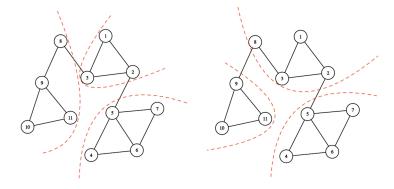


Figure 1: Optimal 3-way partitions of the same graph based on minimum ψ (left) and minimum ϕ (right) respectively.

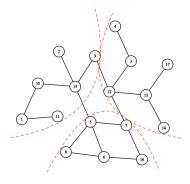


Figure 2: The above 3-way partition leads to the optimal value of both conductance functions ψ and ϕ respectively.

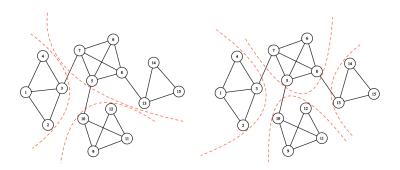


Figure 3: The above 3-way (left) and 4-way (right) partitions of the same graph lead to the optimal value of both conductance functions ψ and ϕ respectively.

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Appendix

A novel proof of the lower bound in Theorem 3.

Define the Rayleigh quotient $R: \mathbb{C}^{|V|} \to \mathbb{R}_+$

$$R(\mathbf{y}) = \frac{\mathbf{y}^{\dagger} \mathbf{L} \mathbf{y}}{\mathbf{v}^{\dagger} \mathbf{D} \mathbf{y}} \tag{6}$$

where \mathbf{y}^{\dagger} is the conjugate transpose of the complex vector \mathbf{y} , \mathbf{L} is the laplacian matrix, and \mathbf{D} is the degree matrix of the graph G.

Define $\mathbf{y}_{\mathscr{S}_k} \in \mathbb{C}^{|V|}$ using $\mathscr{S}_k = \{S_1, S_2, ..., S_k\}$ as follows:

$$\mathbf{y}_{\mathscr{S}_k}(u) = \frac{\omega^i}{vol(S_i)}, \text{ if } u \in S_i \subseteq V$$
 (7)

where ω is the k^{th} root of unity.

The second largest eigenvalue (λ_2) of the normalized laplacian matrix of $G(\mathcal{L})$ can be computed as:

$$\lambda_2 = \min_{\mathbf{y}: \mathbf{y} \neq 0, \mathbf{y}^{\dagger} \mathbf{d} = 0} R(\mathbf{y}) \tag{8}$$

It can be seen that $\mathbf{y}_{\mathscr{S}_k}^{\dagger} \mathbf{d} = 0$:

$$\mathbf{y}_{\mathscr{S}_{k}}^{\dagger} \mathbf{d} = \sum_{u \in V} \overline{\mathbf{y}_{\mathscr{S}_{k}}(u)} \cdot d_{u}$$

$$\implies \mathbf{y}_{\mathscr{S}_{k}}^{\dagger} \mathbf{d} = \sum_{i=1}^{k} \sum_{u \in S_{i}} \frac{\overline{\omega^{i}}}{vol(S_{i})} \cdot d_{u}$$

$$\implies \mathbf{y}_{\mathscr{S}_{k}}^{\dagger} \mathbf{d} = \sum_{i=1}^{k} \frac{\overline{\omega^{i}}}{vol(S_{i})} \cdot \left(\sum_{u \in S_{i}} d_{u}\right)$$

$$\implies \mathbf{y}_{\mathscr{S}_{k}}^{\dagger} \mathbf{d} = \sum_{i=1}^{k} \frac{\overline{\omega^{i}}}{vol(S_{i})} \cdot vol(S_{i})$$

$$\implies \mathbf{y}_{\mathscr{S}_{k}}^{\dagger} \mathbf{d} = \sum_{i=1}^{k} \overline{\omega^{i}}$$

$$\implies \mathbf{y}_{\mathscr{S}_k}^{\dagger} \mathbf{d} = 0 \tag{9}$$

Since, $\mathbf{y}_{\mathscr{S}_k} \neq 0$ and $\mathbf{y}_{\mathscr{S}_k}^{\dagger} \mathbf{d} = 0$:

$$R(\mathbf{y}_{\mathscr{S}_k}) \geq \min_{\mathbf{y}: \ \mathbf{y} \neq \mathbf{0}, \ \mathbf{y}^\dagger \mathbf{d} = \mathbf{0}} R(\mathbf{y})$$

The RHS is the second smallest eigenvalue of \mathcal{L} (from (8)):

$$\implies R(\mathbf{y}_{\mathscr{S}_h}) \ge \lambda_2 \tag{10}$$

Computing $R(\mathbf{y}_{\mathscr{S}_k})$:

$$R(\mathbf{y}_{\mathscr{S}_k}) = \frac{(\mathbf{y}_{\mathscr{S}_k})^{\dagger} \mathbf{L} (\mathbf{y}_{\mathscr{S}_k})}{(\mathbf{y}_{\mathscr{S}_k})^{\dagger} \mathbf{D} (\mathbf{y}_{\mathscr{S}_k})}$$
(11)

Computing $(\mathbf{y}_{\mathscr{S}_k})^{\dagger} \mathbf{L} (\mathbf{y}_{\mathscr{S}_k})$:

$$(\mathbf{y}_{\mathscr{S}_{k}})^{\dagger} \mathbf{L} (\mathbf{y}_{\mathscr{S}_{k}}) = \sum_{uv \in E} ||\mathbf{y}_{\mathscr{S}_{k}}(u) - \mathbf{y}_{\mathscr{S}_{k}}(v)||^{2}$$

$$\Rightarrow (\mathbf{y}_{\mathscr{S}_{k}})^{\dagger} \mathbf{L} (\mathbf{y}_{\mathscr{S}_{k}}) = \sum_{i < j} \sum_{\substack{uv \in E \\ uv \in S_{i} \times S_{j}}} \left| \left| \frac{\omega^{i}}{vol(S_{i})} - \frac{\omega^{j}}{vol(S_{j})} \right| \right|^{2}$$

$$\Rightarrow (\mathbf{y}_{\mathscr{S}_{k}})^{\dagger} \mathbf{L} (\mathbf{y}_{\mathscr{S}_{k}}) = \sum_{i < j} \left(\left| \left| \frac{\omega^{i}}{vol(S_{i})} - \frac{\omega^{j}}{vol(S_{j})} \right| \right|^{2} \cdot \sum_{\substack{uv \in E \\ uv \in S_{i} \times S_{j}}} 1 \right)$$

$$\Rightarrow (\mathbf{y}_{\mathscr{S}_{k}})^{\dagger} \mathbf{L} (\mathbf{y}_{\mathscr{S}_{k}}) \leq \left(\sum_{i < j} \left| \left| \frac{\omega^{i}}{vol(S_{i})} - \frac{\omega^{j}}{vol(S_{j})} \right| \right|^{2} \right) \cdot \left(\sum_{i < j} \sum_{\substack{uv \in E \\ uv \in S_{i} \times S_{j}}} 1 \right)$$

$$\sum_{i < j} \sum_{\substack{uv \in E \\ uv \in S_{i} \times S_{j}}} 1 = \frac{1}{2} \cdot \sum_{i \neq j} \sum_{\substack{uv \in E \\ uv \in S_{i} \times S_{j}}} 1$$

$$\Rightarrow \sum_{i < j} \sum_{\substack{uv \in E \\ uv \in S_{i} \times S_{j}}} 1 = \frac{1}{2} \cdot \sum_{i} cut(S_{i})$$

$$(13)$$

From (12) and (13):

$$(\mathbf{y}_{\mathscr{S}_k})^{\dagger} \mathbf{L} (\mathbf{y}_{\mathscr{S}_k}) \leq \left(\sum_{i < j} \left| \left| \frac{\omega^i}{vol(S_i)} - \frac{\omega^j}{vol(S_j)} \right| \right|^2 \right) \cdot \frac{1}{2} \cdot \sum_i cut(S_i)$$

For $a, b \in \mathbb{C}$, $||a - b||^2 \le (||a|| + ||b||)^2$:

$$\implies (\mathbf{y}_{\mathscr{S}_{k}})^{\dagger} \mathbf{L} (\mathbf{y}_{\mathscr{S}_{k}}) \leq \left(\sum_{i < j} \left(\left\| \frac{\omega^{i}}{vol(S_{i})} \right\| + \left\| \frac{\omega^{j}}{vol(S_{j})} \right\| \right)^{2} \right) \cdot \frac{1}{2} \cdot \sum_{i} cut(S_{i})$$

$$\implies (\mathbf{y}_{\mathscr{S}_{k}})^{\dagger} \mathbf{L} (\mathbf{y}_{\mathscr{S}_{k}}) \leq \left(\sum_{i < j} \left(\frac{1}{vol(S_{i})} + \frac{1}{vol(S_{j})} \right)^{2} \right) \cdot \frac{1}{2} \cdot \sum_{i} cut(S_{i})$$

$$(14)$$

Computing $(\mathbf{y}_{\mathscr{S}_k})^{\dagger} \mathbf{D} (\mathbf{y}_{\mathscr{S}_k})$:

$$(\mathbf{y}_{\mathscr{S}_k})^{\dagger} \mathbf{D} (\mathbf{y}_{\mathscr{S}_k}) = \sum_{u \in V} d_u ||\mathbf{y}_{\mathscr{S}_k}(u)||^2$$

$$\Rightarrow (\mathbf{y}_{\mathscr{S}_{k}})^{\dagger} \mathbf{D} (\mathbf{y}_{\mathscr{S}_{k}}) = \sum_{i=1}^{k} \sum_{u \in S_{i}} d_{u} \left\| \frac{\omega^{i}}{vol(S_{i})} \right\|^{2}$$

$$\Rightarrow (\mathbf{y}_{\mathscr{S}_{k}})^{\dagger} \mathbf{D} (\mathbf{y}_{\mathscr{S}_{k}}) = \sum_{i=1}^{k} \sum_{u \in S_{i}} d_{u} \left(\frac{1}{vol(S_{i})} \right)^{2}$$

$$\Rightarrow (\mathbf{y}_{\mathscr{S}_{k}})^{\dagger} \mathbf{D} (\mathbf{y}_{\mathscr{S}_{k}}) = \sum_{i=1}^{k} vol(S_{i}) \left(\frac{1}{vol(S_{i})} \right)^{2}$$

$$\Rightarrow (\mathbf{y}_{\mathscr{S}_{k}})^{\dagger} \mathbf{D} (\mathbf{y}_{\mathscr{S}_{k}}) = \sum_{i=1}^{k} \frac{1}{vol(S_{i})}$$
(15)

Let $Sum_1 = \sum_i \frac{1}{vol(S_i)}$ and let $Sum_2 = \sum_i \frac{1}{vol(S_i)^2}$. Then:

$$\sum_{i \le j} \left(\frac{1}{vol(S_i)} + \frac{1}{vol(S_j)} \right)^2 = (k-2) \cdot Sum_2 + (Sum_1)^2, \text{ where } k = |\mathcal{S}|$$
 (16)

Finding an upper bound on $(k-2) \cdot Sum_2$ as follows:

$$Sum_{2} \leq Sum_{1} \cdot \max_{i} \left(\frac{1}{vol(S_{i})}\right)$$

$$\implies (k-2) \cdot Sum_{2} \leq (k-2) \cdot Sum_{1} \cdot \max_{i} \left(\frac{1}{vol(S_{i})}\right)$$
(17)

Finding an upper bound on $(Sum_1)^2$ as follows:

$$Sum_{1} \leq k \cdot \max_{i} \left(\frac{1}{vol(S_{i})} \right)$$

$$\implies (Sum_{1})^{2} \leq k \cdot Sum_{1} \cdot \max_{i} \left(\frac{1}{vol(S_{i})} \right)$$
(18)

Adding (17) and (18):

$$(k-2) \cdot Sum_2 + (Sum_1)^2 \le (2k-2) \cdot Sum_1 \cdot \max_i \left(\frac{1}{vol(S_i)}\right)$$
(19)

From (14), (16), and (19):

$$(\mathbf{y}_{\mathscr{S}_{k}})^{\dagger} \mathbf{L} (\mathbf{y}_{\mathscr{S}_{k}}) \leq (2k - 2) \cdot Sum_{1} \cdot \max_{i} \left(\frac{1}{vol(S_{i})}\right) \cdot \frac{1}{2} \cdot \sum_{i} cut(S_{i})$$

$$\implies (\mathbf{y}_{\mathscr{S}_{k}})^{\dagger} \mathbf{L} (\mathbf{y}_{\mathscr{S}_{k}}) \leq (k - 1) \cdot \left(\sum_{i} \frac{1}{vol(S_{i})}\right) \cdot \max_{i} \left(\frac{1}{vol(S_{i})}\right) \cdot \sum_{i} cut(S_{i})$$
(20)

From (15) and (20)

$$\frac{(\mathbf{y}_{\mathscr{S}_{k}})^{\dagger} \mathbf{L} (\mathbf{y}_{\mathscr{S}_{k}})}{(\mathbf{y}_{\mathscr{S}_{k}})^{\dagger} \mathbf{D} (\mathbf{y}_{\mathscr{S}_{k}})} \leq (k-1) \cdot \max_{i} \left(\frac{1}{vol(S_{i})}\right) \cdot \sum_{i} cut(S_{i})$$

$$\Longrightarrow R(\mathbf{y}_{\mathscr{S}_{k}}) \leq (k-1) \cdot \frac{\sum_{i} cut(S_{i})}{\min_{i} vol(S_{i})}$$
(21)

From (10) and (21):

$$\frac{\lambda_2}{k \cdot (k-1)} \le \frac{1}{k} \cdot \frac{\sum_i cut(S_i)}{\min_i vol(S_i)}$$

$$\implies \frac{\lambda_2}{k \cdot (k-1)} \le \psi(\mathscr{S}_k) \tag{22}$$

Therefore, we have found a lower bound on the generalized conductance function.