SDP Notes

The Ratio Cut Problem

Given a fully connected, undirected similarity graph $G = (V, E)$ represented by weight matrix W, and known number of clusters/communities k, ratio cut partitions the graph by minimizing the objective function:

$$\arg\min_H \operatorname{Tr}(H^\top LH)$$

where L is the unnormalized combinatorial Laplacian matrix $L = D - W$, D is the diagonal degree matrix $d_{ii} = \sum_j w_{ij}$, and $H \in \mathbb{R}^{n \times k}$ is restricted to the form $h_{ij} = \begin{cases} n_j^{-1/2} & \text{vertex } i \text{ is in cluster } j \\ 0 & \text{else} \end{cases}$

This problem is NP-hard, which brings us to ...

Spectral Clustering

Note that $H^\top H = I$. So instead of restricting H to a cluster membership matrix, we just restrict H such that $H^\top H = I$. Then $H = \begin{bmatrix} v_0 & v_1 & \cdots & v_{k-1} \end{bmatrix}$, or the matrix of k eigenvectors that correspond to the smallest k eigenvalues. Since this does not provide cluster memberships, the first k eigenvectors are then treated as an embedding of the graph G and k-means clustering is then applied (e.g., using Lloyd's algorithm) to obtain cluster memberships.[1]

However, there isn't much theoretical justification for this approach, nor are there any guarantees that it will result in a clustering that minimizes the ratio cut objective, which brings us to ...

Semidefininte Programming Approach

Ling and Strohmer[2] showed that under certain conditions, the ratio cut problem can be solved exactly using semidefinite programming.

First, we note that $\operatorname{Tr}(H^\top LH) = \operatorname{Tr}(LHH^\top)$. Let us denote $Z = HH^\top$. We can see that $z_{ij} = n_k^{-1}$ if vertices i and j both belong to the same cluster (where n_k is the size of that cluster), otherwise it is 0. We can then note that $\operatorname{Tr}(Z) = k$, the number of clusters, and Z is positive semidefinite of rank k. We also note that $Ze = e$ where e is a constant vector.

The SDP approach relaxes these constraints on Z but keeps more constraints than the spectral clustering approach. More formally, the SDP ratio cut algorithm is as follows:

1. Solve $\arg\min_Z \operatorname{Tr}(LZ)$ subject to
   - Z is positive semidefinite
   - $Z \geq 0$ element-wise
   - $\operatorname{Tr}(Z) = k$
   - $Ze = e$
2. Use the solution to the above to obtain cluster memberships.

The paper does not make it clear how to actually solve the semidefinite programming problem or how to recover cluster memberships from Z, since we are not guaranteed to obtain the "correct" form of Z using this method.

[1] This is almost (but not quite) the same as performing kernel k-means clustering using the Moore-Penrose pseudoinverse of L as a kernel matrix.

[2] https://arxiv.org/abs/1806.11429

Possibly Interesting Question

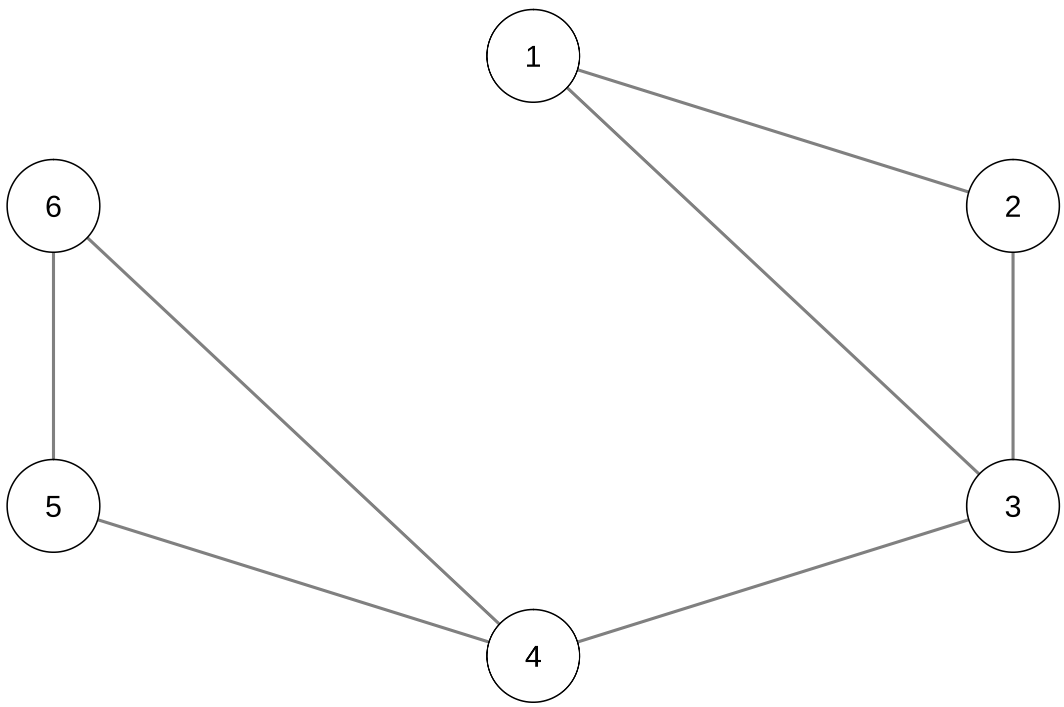
We previously noted that the spectral clustering approach to ratio cut is almost equivalent to kernel k-means using the pseudoinverse of L as a kernel matrix. One problem that we have been trying to solve is under what conditions does kernel k-means provide the optimal ratio cut clustering. Similarly, we might be interested in a kernel k-means version of the semidefinite programming approach:

Let $L^\dagger$ be the pseudoinverse of L. Solve $\arg\max_Z \operatorname{Tr}(L^\dagger Z)$ subject to

- Z is positive semidefinite
- $Z \geq 0$ element-wise
- $\operatorname{Tr}(Z) = k$
- $Ze = e$

Some Examples

We will begin with a very simple graph with six vertices:



It is clear (and easy to verify) that cutting the $3-4$ edge is optimal under the ratio cut objective. Using the semidefinite programming method:

```
$Z
      [,1]  [,2]  [,3]  [,4]  [,5]  [,6]
[1,] 0.333 0.333 0.333 0.000 0.000 0.000
[2,] 0.333 0.333 0.333 0.000 0.000 0.000
[3,] 0.333 0.333 0.333 0.000 0.000 0.000
[4,] 0.000 0.000 0.000 0.333 0.333 0.333
[5,] 0.000 0.000 0.000 0.333 0.333 0.333
[6,] 0.000 0.000 0.000 0.333 0.333 0.333

$clustering
```

```
[1] 1 1 1 2 2 2
```

We in fact get the exact solution to Z. The clustering here is based on a spectral decomposition of Z, which can have up to $n-1$ nonzero eigenvectors (in this case we only have two). k-means is applied to this embedding.

We can also try the kernel k-means approach:

```
$Z
      [,1]  [,2]  [,3]  [,4]  [,5]  [,6]
[1,] 0.333 0.333 0.333 0.000 0.000 0.000
[2,] 0.333 0.333 0.333 0.000 0.000 0.000
[3,] 0.333 0.333 0.333 0.000 0.000 0.000
[4,] 0.000 0.000 0.000 0.333 0.333 0.333
[5,] 0.000 0.000 0.000 0.333 0.333 0.333
[6,] 0.000 0.000 0.000 0.333 0.333 0.333

$clustering
[1] 2 2 2 1 1 1
```

And in fact we get identical results as before for both Z and the clustering.

Let's try the epsilon graph example from the text. Recall that the graph Laplacian is of the form $\begin{bmatrix} \epsilon & -\epsilon & 0 & 0 \\ -\epsilon & 1+\epsilon & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 1 \end{bmatrix}$. Ratio cut and kernel k-means gave different answers when $\epsilon \in (0.6, 0.75)$.

Plugging in $\epsilon = 0.6$, the SDP method for ratio cut gives:

```
$Z
      [,1]  [,2]  [,3]  [,4]
[1,] 0.777 0.223 0.000 0.000
[2,] 0.223 0.355 0.275 0.147
[3,] 0.000 0.275 0.370 0.355
[4,] 0.000 0.147 0.355 0.498

$clustering
[1] 1 2 2 2
```

While the SDP method for kernel k-means gives:

```
$Z
      [,1]  [,2]  [,3]  [,4]
[1,] 0.683 0.317 0.000 0.000
[2,] 0.317 0.394 0.211 0.077
[3,] 0.000 0.211 0.394 0.394
[4,] 0.000 0.077 0.394 0.528

$clustering
[1] 1 1 2 2
```

Plugging in $\epsilon = .7$:

```
$Z
      [,1]  [,2]  [,3]  [,4]
[1,] 0.708 0.292 0.000 0.000
[2,] 0.292 0.368 0.243 0.096
[3,] 0.000 0.243 0.389 0.368
```

```
[4,] 0.000 0.096 0.368 0.535

$clustering
[1] 2 2 1 1
```

While the SDP method for kernel k-means gives:

```
$Z
      [,1]  [,2]  [,3]  [,4]
[1,] 0.581 0.419 0.000 0.000
[2,] 0.419 0.439 0.122 0.020
[3,] 0.000 0.122 0.439 0.439
[4,] 0.000 0.020 0.439 0.541

$clustering
[1] 2 2 1 1
```

So while we can get SDP ratio cut and SDP kernel k-means to disagree, the conditions are not identical to when this happens for the spectral clustering methods.