Foundations of Spectral Clustering

Dong Li

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Motivation

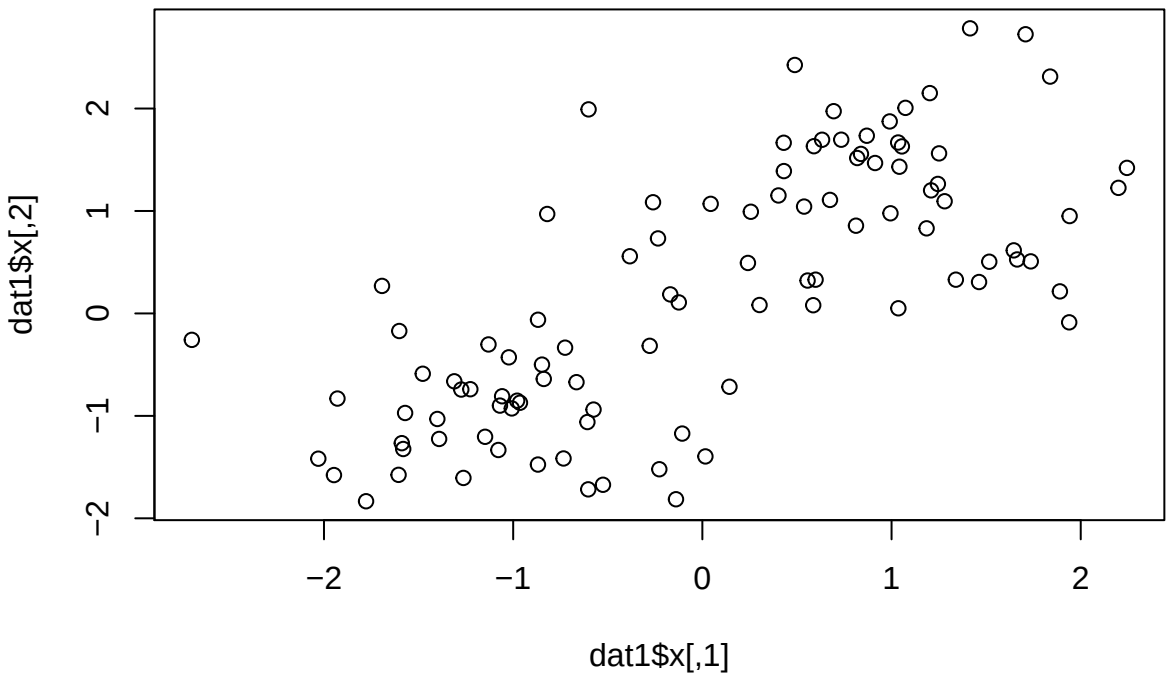
Recently we read a Nature paper which adopts spectral clustering as the main method to find higher-order connectivity patterns. The efficiency and scalability of their algorithm are impressive. And We also found that the best player in this year's Disease Module Identification DREAM Challenge uses spectral clustering as one of their main techniques to identify modules, which achieved the best overall performance at all FDR levels. Check their write-up: A Double Spectral Approach to DREAM 11 Subchallenge 3.

As a classical clustering method, spectral techniques are still promising. The basic questions remain as: what is spectral clustering and why it works?

A starter dish about clustering

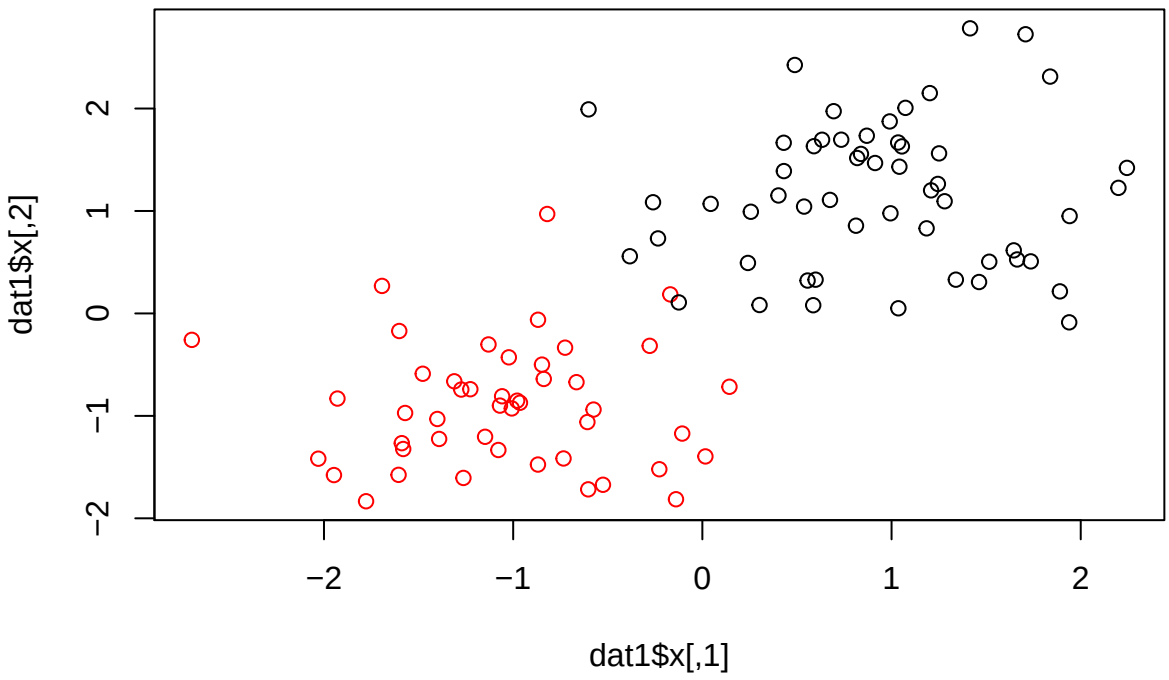
Before we step into spectral clustering, let's look at a simple example about clustering. Image we have a collection of two-dimensional data points looks like,

```
library(mlbench)
n = 100
k = 2
dat1 = mlbench.2dnormals(n, cl=k, r=sqrt(k), sd=0.7)
plot(dat1$x,col=rep(1,n))
```



How many clusters are there? It is easy for human to say

```
plot(dat1$x,col=dat1$classes)
```



But how can we make the program know? We may need classical K-means algorithm. The idea of k-means is quite straightforward:

- 1) randomly picking k nodes as centroids,
- 2) assign each data points to the centroids which is the most "close",
- 3) calculated the new centroids based on previous assignment and
- 4) repeat 2-3 until the centroids keep unchanged.

Code for 2) Assignment and 3) Update centroids:

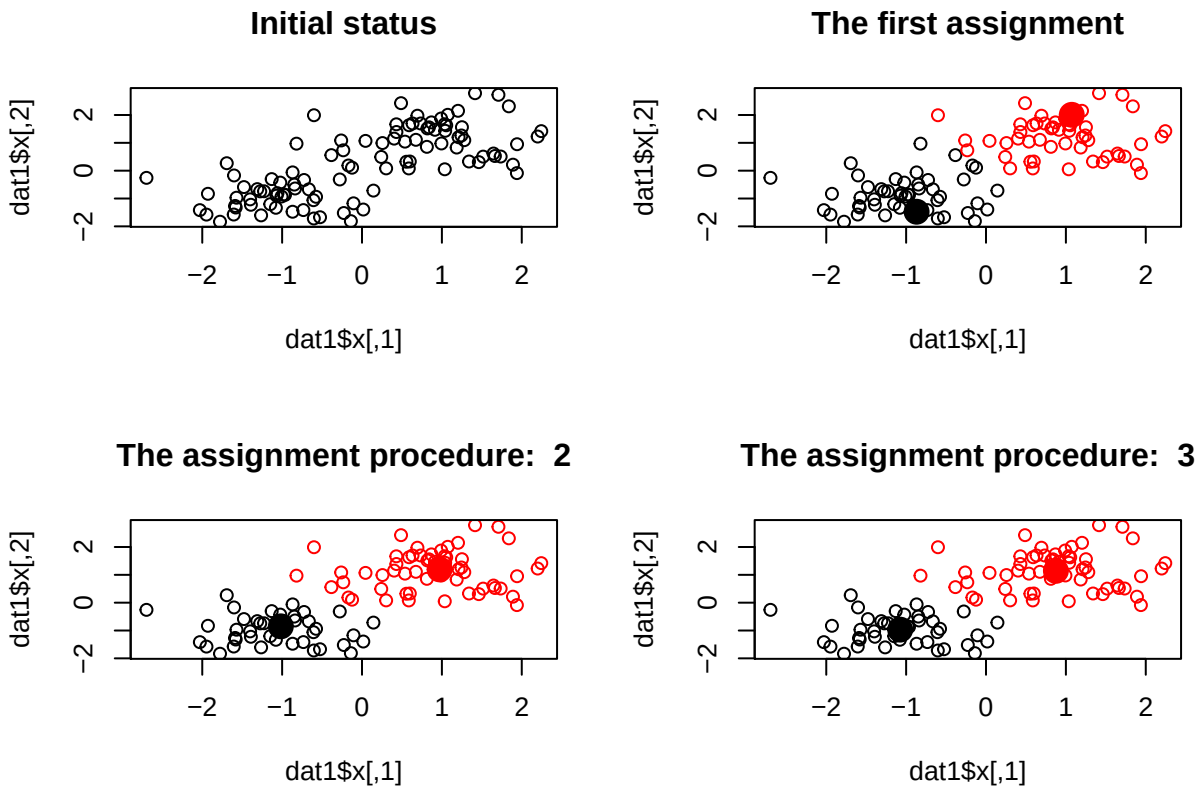
```
# Assign cluster labels given centroidids
Assigment <- function(dat,centroidids){
    n <- dim(dat)[1]
    k <- dim(centroidids)[1]
    classes <- rep(1,n)

    for(i in 1:n){
        #mindist <- dist(rbind(dat[i,],centroidids[1]))
        mindist <- norm(as.matrix(dat[i,]-centroidids[1]), type="F")
        for(j in 2:k){
            currentdis = norm(as.matrix(dat[i,]-centroidids[j]), type="F")
            if( currentdis < mindist){
                mindist = currentdis
                classes[i] = j
```

```
            }
        }
    }
    classes
}

# Update centroidids given cluster labels
Update <- function(dat,classes,k){
    l = dim(dat)[2]
    centroidids <- matrix(0, nrow=k,ncol=l)
    for(i in 1:k){
        centroidids[i,] =  colMeans(dat[which(classes==i),])
    }
    centroidids
}
```

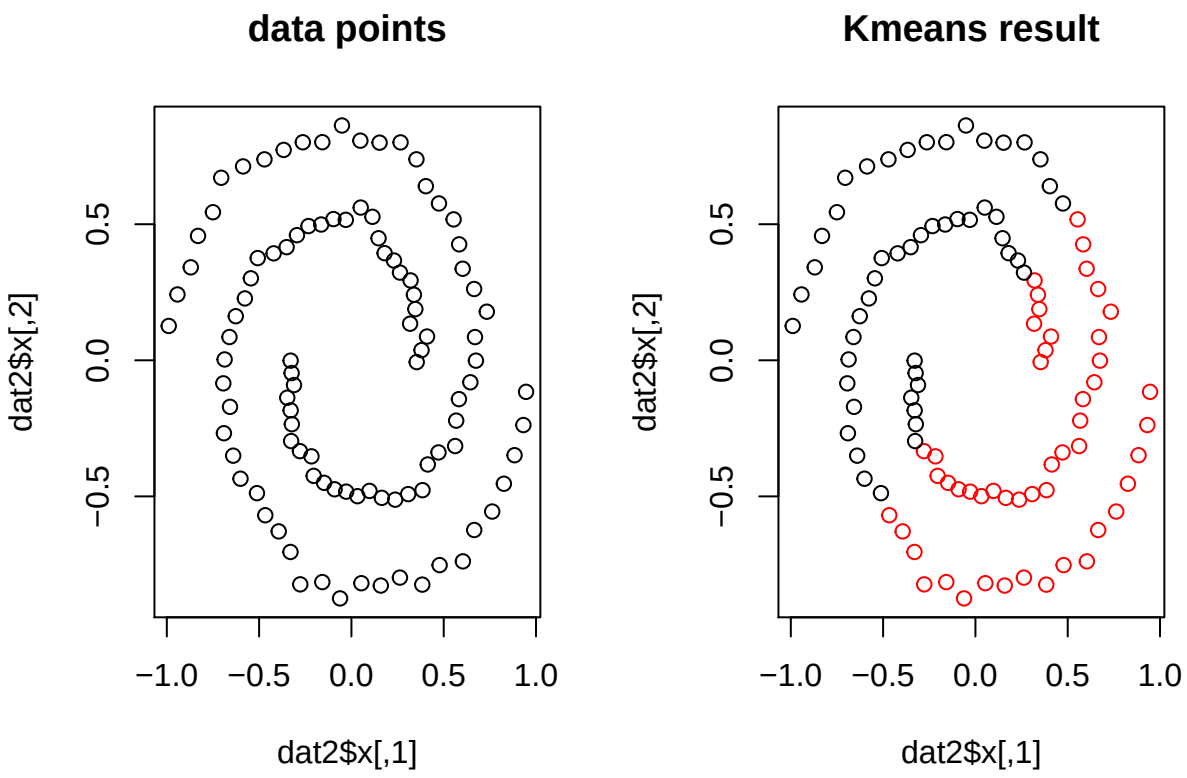
The basic k-means seems to work well in previous example. We can see the procedure of how centroids move step by step:



But when the data points are not so straightforward (linearly separable), such as spirals, where k-means may fail:

```
dat2 <- mlbench.spirals(100,1,0.025)
par(mfrow=c(1,2))
plot(dat2$x)
title('data points')
```

```r
#we call the system function kmeans this time
km <- kmeans(dat2$x, centers=k)
plot(dat2$x, col=km$cluster)
title('Kmeans result')
```



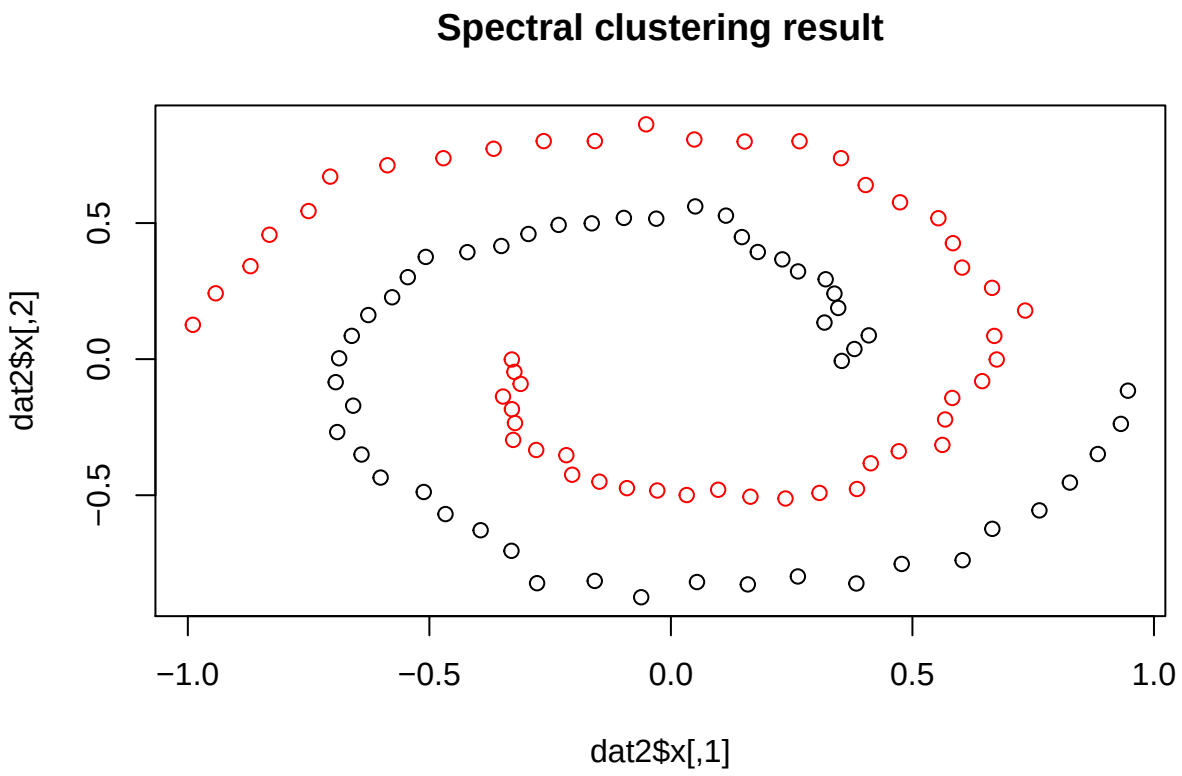
We will see spectral clustering can work well here.

Spectral clustering algorithms

Spectral clustering makes use of spectrum(eigenvalues) of the similarity matrix to perform data analysis. One simple form of the algorithm goes like

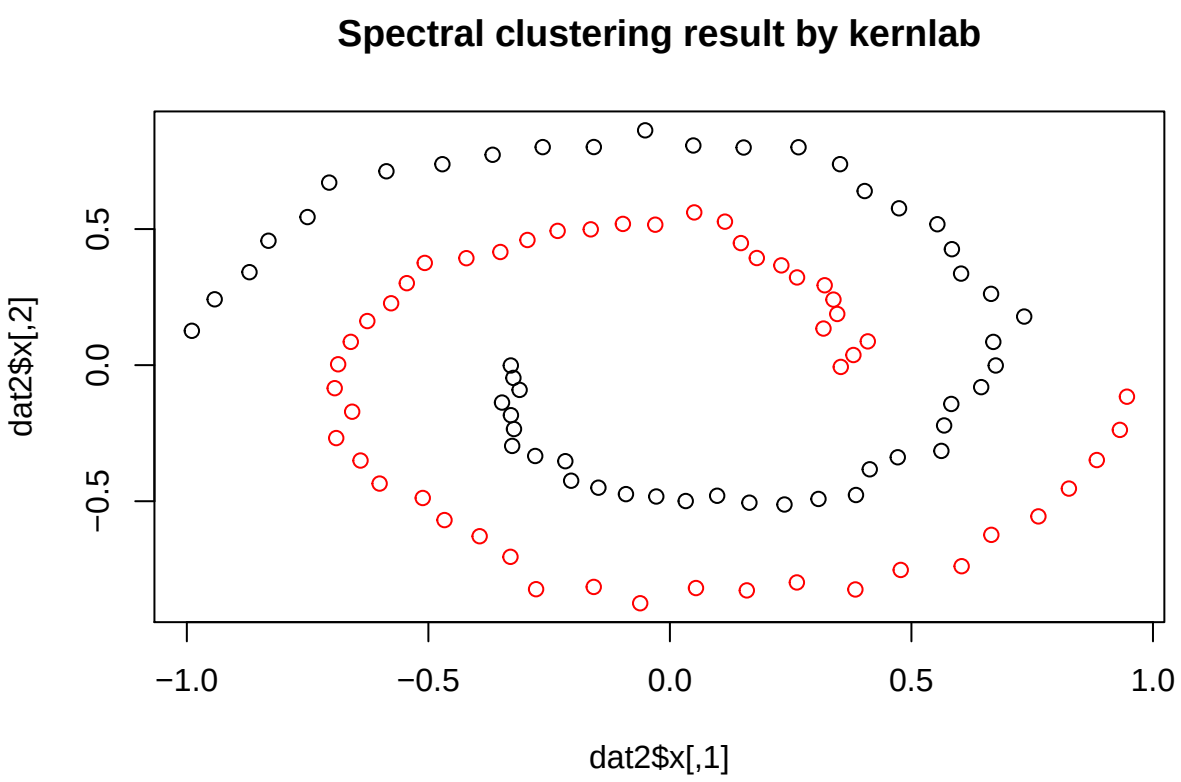
- Make the affinity matrix A based on the similarity matrix W.
- Make the diagonal matrix D where $D_{ii} = \sum_j A_{ij}$, and the unnormalized Laplacian matrix $L = D - A$ or normalized Laplacian matrix $L = D^{-1/2}AD^{-1/2}$.
- Find the first k eigenvectors $x_1, x_2, ...x_k$ of L and form the new matrix $X = [x_1 x_2 ... x_k] \in \mathbb{R}^{n \times k}$.
- Conduct K-means on X.

Note that the affinity matrix is not always the similarity matrix W. For some problem we need to consider the local neighborhood relationships. k-nearest neighboor filter is a common choice:



And all these can be done in one line with package kernlab.

```
library(kernlab)
skm=specc(dat2$x,centers=2)
plot(dat2$x, col=skm)
title('Spectral clustering result by kernlab')
```



Why spectral clustering works?

At the first sight you may feel amazing. Why it works? Why we pick exactly k eigenvectors and why they are separable under this representation? Following the logic of Luxburg's Tutorial, the principle of explaining why Eigendecomposition can be used to do clustering is to **establish an equivalence between Eigendecomposition based procedure and clustering data points**. We only explore it from the Graph cut perspective based on normalized Laplacian.

The essence of clustering is to separate data points based on their similarities. Given the similarity graph (where nodes are data points and edges are similarities) of these points, it aims to find a partition that edges within the same cluster are dense and between different clusters are sparse. This problem has been intensively studied in graph theory.

Check Cut to distinguish similar concepts of cut, cut-set and Minimum cut. Given the adjacency matrix W of a graph $G = (V, E)$, we define the following metric for two disjoint subsets $A, B \in V$:

$$cut(A, B) = \sum_{i \in A, j \in B} w_{ij}$$

and $\bar{A}$ as the complement of A. For given k clusters, we want to find a partition $A_1, A_2, ...A_k$ that minimizes

$$Cut(A_1, A_2, ...A_k) = \frac{1}{2} \sum_{i=1}^{k} cut(A_i, \bar{A}_i)$$

. But simply minizing this metric would lead to large clusters. Several improvements were proposed and we

mainly discuss normalized cut Ncut:

$$Ncut(A,B) = \sum_{i=1}^{k} \frac{cut(A_i, \bar{A}_i)}{vol(A_i)}$$

where $vol(A) = \sum_{i \in A, j} w_{i,j} = \sum_{i \in A} d_i$ and d_i is the connectivity (degree) of i.

Next we want to derive normalized spectral clustering as relaxation of minimizing Ncut. Considering the simplest case When $k = 2$, there are only A and $\bar{A}$, we define the cluster indicator f (this is the key idea) as

$$f_i = \begin{cases} \sqrt{\frac{vol(\bar{A})}{vol(A)}} & if \quad v_i \in A \\ -\sqrt{\frac{vol(A)}{vol(\bar{A})}} & if \quad v_i \in \bar{A} \end{cases}$$

Note that $f^T D\mathbf{1} = 0$. As we know $D_{ii} = d_i$, thus

$$\begin{aligned} &\textstyle\sum_i f_i d_i = \sqrt{vol(\bar{A})/vol(A)} \sum_{i \in A} d_i - \sqrt{vol(A)/vol(\bar{A})} \sum_{j \in \bar{A}} d_j \\ &= \sqrt{vol(\bar{A})/vol(A)} vol(A) - \sqrt{vol(A)/vol(\bar{A})} vol(\bar{A}) = 0 \end{aligned}$$

. And we also have $f'Df = vol(V)$ since

$$\begin{aligned} &f'Df = \textstyle\sum_i f_i^2 d_i = \sum_{i \in A} d_i \frac{vol(\bar{A})}{vol(A)} + \sum_{i \in \bar{A}} d_i \frac{vol(A)}{vol(\bar{A})} \\ &= vol(\bar{A}) + vol(A) = vol(V) \end{aligned}$$

For every f we have $f'Lf = 1/2 \sum_{ij} (f_i - f_j)^2$, and for the specific f defined above, we have

$$\begin{aligned} &f'Lf = \tfrac{1}{2} \textstyle\sum_{i \in A, j \in \bar{A}} w_{ij} \Big(\sqrt{\frac{vol(\bar{A})}{vol(A)}} + \sqrt{\frac{vol(A)}{vol(\bar{A})}} \Big)^2 + \frac{1}{2} \sum_{i \in \bar{A}, j \in A} w_{ij} \Big(- \sqrt{\frac{vol(A)}{vol(\bar{A})}} - \sqrt{\frac{vol(\bar{A})}{vol(A)}} \Big)^2 \\ &= cut(A, \bar{A}) \Big(\frac{vol(A)}{vol(\bar{A})} + \frac{vol(\bar{A})}{vol(A)} + 2 \Big) \\ &= cut(A, \bar{A}) \Big(\frac{vol(A) + vol(\bar{A})}{vol(\bar{A})} + \frac{vol(\bar{A}) + vol(A)}{vol(A)} + 2 \Big) \\ &= vol(V) Ncut(A, \bar{A}) \end{aligned}$$

Because $vol(V)$ is constant for given graph, the equivalence problem of minimize Ncut is to minimize $f'Lf$ w.r.t f. Unfortunately it is a discrete optimization problem.

If we relax the vector f to real number space we have the following optimization problem

$$\min_{f \in \mathbb{R}^n} f'Lf \quad s.t. \quad f^T D \perp \mathbb{1}, f'Df = vol(V)$$

Furthermore we make $g = D^{1/2} f$, the problem becomes

$$\min_{g \in \mathbb{R}^n} g' L_{sym} g \quad s.t. \quad g \perp D^{1/2}\mathbb{1}, \|g\|^2 = vol(V)$$

where $L_{sym} = D^{-1/2} L D^{-1/2}$. According to Rayleigh quotient, the solution is given by the second eigenvector of L_{sym}. That means as long as we get f by eigenvector of L_{sym}, we get a partition which make minimize Ncut thus get the clusters. Refer to Luxburg's Tutorial when $k > 2$.

References

This document is written in R Markdown. Want to write one like this? See Writing reproducible reports in R.

A close topic was given by João Neto at Spectral Clustering.

A nice tutorial of spectral clustering was given by Luxburg at A Tutorial on Spectral Clustering.

A popular Chinese machine learning blog by pluskid also contains spectral clustering.