Spectral Method for Modularity Maximization

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Problem . Maximize modularity Q:

$$Q = \frac{1}{2m} \sum_{ij} \left[A_{ij} - \frac{k_i k_j}{2m} \right] \delta_{g_i g_j}, \tag{1}$$

where

$$\delta_{g_i g_j} = \frac{1}{2} \left(s_i s_j + 1 \right) \tag{2}$$

and

$$s_i = \begin{cases} +1, & \text{if vertex } i \text{ belongs to group 1} \\ -1, & \text{if vertex } i \text{ belongs to group 2} \end{cases} \tag{3}$$

Solution.

Take $\delta_{g_i g_j} = \frac{1}{2} \left(s_i s_j + 1 \right)$ to equation (1). Then

$$Q = \frac{1}{4m} \sum_{ij} \left[A_{ij} - \frac{k_i k_j}{2m} \right] \left(s_i s_j + 1 \right). \tag{4}$$

Define the quantity B, called modularity matrix

$$B_{ij} = A_{ij} - \frac{k_i k_j}{2m}. \tag{5}$$

The sums of all its rows and columns are zero:

$$\begin{aligned} \sum_j B_{ij} &= \sum_j A_{ij} - \sum_j \frac{k_i k_j}{2m} && (6) \\ &= k_i - 2m \frac{k_i}{2m} && (7) \\ &= 0 && (8) \end{aligned}$$

Use substitute B_{ij} for A_{ij}:

$$Q = \frac{1}{4m} \sum_{ij} B_{ij} \left(s_i s_j + 1 \right). \tag{9}$$

$$= \frac{1}{4m} \sum_{ij} B_{ij} s_i s_j + \frac{1}{4m} \sum_{ij} B_{ij} \tag{10}$$

$$= \frac{1}{4m} \sum_{ij} B_{ij} s_i s_j \tag{11}$$

Our task is to maximize Q over the possible choices of the s_i.
Relax s_i to any real value:

$$s_i \in \mathbb{R}$$

Use constrain:

$$\sum_i k_i s_i^2 = 2m, \tag{12}$$

where $\sum_i k_i = 2m$. The original vector s is mapped to the boundary of a hyper ellipsoid.
To make the problem simple, we define Q' as the objective function:

$$Q' = \sum_{ij} B_{ij} s_i s_j \tag{13}$$

Based on the theorem of the Lagrange multiplier [P5. Theorem Lagrange multiplier], we define Lagrange function:

$$F = \sum_{ij} B_{ij} s_i s_j + \lambda \left(2m - \sum_i k_i s_i^2 \right) \tag{14}$$

when all s_i and λ satisfy

$$\begin{cases} \frac{\partial F}{\partial s_i} = 0 \\ \frac{\partial F}{\partial \lambda} = 0 \end{cases} \tag{15}$$

vector $\mathbf{s} = (s_1, s_2, ...)$ will be the stationary point.

$$\frac{\partial F}{\partial s_i} = \frac{\partial}{s_i} \left(\sum_{ij} B_{ij} s_i s_j + \lambda \left(2m - \sum_i k_i s_i^2 \right) \right) = 0 \tag{16}$$

$$2 \sum_j B_{ij} s_j - 2\lambda k_i s_i = 0 \tag{17}$$

Then,

$$\sum_j B_{ij} s_j = \lambda k_i s_i \tag{18}$$

or, in matrix notation,

$$\mathbf{Bs} = \lambda \mathbf{Ds} \tag{19}$$

where $\mathbf{D}$ is the diagonal matrix with elements equal to the vertex degrees $\mathbf{D}_{ii} = k_i$

Use the adjacency matrix $\mathbf{A}$ to substitute modularity matrix $\mathbf{B}$. Then, according to equation (5),

$$\sum_j \left(A_{ij} - \frac{k_i k_j}{2,}\right) s_j = \lambda k_i s_i \tag{20}$$

$$\sum_j A_{ij} s_j = k_i \left(\lambda s_i + \sum_j \frac{k_j}{2m} s_j\right) \tag{21}$$

or, in matrix notation,

$$\mathbf{As} = \mathbf{D}\left(\lambda \mathbf{s} + \frac{\mathbf{k}^T \mathbf{s}}{2m} \mathbf{1}\right) \tag{22}$$

where $\mathbf{1} = (1, 1, ...)$.

It can be obvious observed that

$$\mathbf{A1}{=}\mathbf{D1}{=}\mathbf{k} \tag{23}$$

Also, for that $\mathbf{A}$, $\mathbf{D}$ are symmetric matrices, we have:

$$\mathbf{A} = \mathbf{A}^T \qquad \mathbf{D} = \mathbf{D}^T \tag{24}$$

And for that $\sum_i k_i = 2m$, we have:

$$\mathbf{k}^T \mathbf{1} = 2m \tag{25}$$

So, equation (22) can be deformed step by step. Let both the left side and right side multiply $\mathbf{1}^T$.

$$\mathbf{1}^T \mathbf{As} = \mathbf{1}^T \mathbf{D}\left(\lambda \mathbf{s} + \frac{\mathbf{k}^T \mathbf{s}}{2m} \mathbf{1}\right) \tag{26}$$

$$(\mathbf{A1})^T \mathbf{s} = (\mathbf{D1})^T \left(\lambda \mathbf{s} + \frac{\mathbf{k}^T \mathbf{s}}{2m} \mathbf{1}\right) \tag{27}$$

$$\mathbf{k}^T\mathbf{s} = \lambda\mathbf{k}^T\left(\mathbf{s} + \frac{\mathbf{k}^T\ \mathbf{s}}{2m}\mathbf{1}\right) \tag{28}$$

$$\mathbf{k}^T\mathbf{s} = \lambda\mathbf{k}^T\mathbf{s} + \frac{\mathbf{k}^T\ \mathbf{s}}{2m}\mathbf{k}^T\mathbf{1} \tag{29}$$

$$\mathbf{k}^T\mathbf{s} = \lambda\mathbf{k}^T\mathbf{s} + \frac{\mathbf{k}^T\ \mathbf{s}}{2m} \times 2m \tag{30}$$

$$\mathbf{k}^T\mathbf{s} = \lambda\mathbf{k}^T\mathbf{s} + \mathbf{k}^T\ \mathbf{s} \tag{31}$$

$$\lambda\mathbf{k}^T\mathbf{s} = 0 \tag{32}$$

Since we are assuming there exists a nontrivial eigenvalue value $\lambda > 0$, we know that $\lambda \neq 0$. Hence

$$\mathbf{k}^T\mathbf{s} = 0 \tag{33}$$

Equation (22) simplifies to

$$\mathbf{A}\mathbf{s} = \lambda\mathbf{D}\mathbf{s} \tag{34}$$

Obviously, $\lambda = 1$ when $\mathbf{s} = \mathbf{1}$ is a solution to this function. But it does not satisfy constrain equation (33). By Perron-Frobenius theorem, $\lambda = 1$ is the most positive eigenvalue. So to maximize Q, we need to use the second positive eigenvalue.

To make it more simple, define:

$$\mathbf{u} = \mathbf{D}^{1/2}\mathbf{s} \tag{35}$$

and use the normalized Laplacian:

$$\mathcal{L} = \mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2} \tag{36}$$

equation (34‘) can be deformed as:

$$\mathcal{L}\mathbf{u} = \lambda\mathbf{u} \tag{37}$$

Because the elements of **s** and **u** have the same sign correspondingly. So the solution of the original maximization problem is the sign of eigenvector **u**, when the eigenvalue is the second positive one.

□

Theorem Lagrange multiplier. Maximize $f(x, y)$, subject to $g(x, y) = c$. We need both f and g to have continuous first partial derivatives. We introduce a new variable λ called a Lagrange multiplier and study the Lagrange function (or Lagrangian) defined by

$$\mathcal{L} = f(x, y) - \lambda\,(g(x, y) - c)$$

where the λ term may be either added or subtracted. If $f(x_0, y_0)$ is a maximum of $f(x, y)$ for the original constrained problem, then there exists λ_0 such that (x_0, y_0, λ_0) is a stationary point for the Lagrange function (stationary points are those points where the partial derivatives of $\mathcal{L}$ are zero).