Modularity-Maximizing Graph Communities via Mathematical Programming

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Modularity Maximization

Given undirected graph $G = (V, E)$, find a clustering $\{C_1, \ldots, C_k\}$ which is a **disjoint** partition of V such that the modularity of the clustering $\mathcal{C}$[1]:

$$\mathcal{Q}(\mathcal{C}) = \frac{1}{2m} \sum_{u,v} (a_{u,v} - \frac{d_u d_v}{2m}) \cdot \delta(\gamma(u), \gamma(v))$$

is **maximized**. Here,

- $a_{u,v} = a_{v,u} = 1$ if $(u, v) \in E$, otherwise 0;
- d_u denotes the degree of any vertex u;
- m is the number of edges in G;
- $\gamma(v)$ denotes the (unique) index of the cluster to which v belongs;
- $\delta(x, y)$ is the Kronecker Delta, which equals to 1 if $x = y$, otherwise 0.

Recent Efforts

- This maximization problem is NP-complete[2];
- Correlation Clustering[3] interprets "partial membership of the same cluster" as a distance metric, group nearby ones together;
- Spectral Clustering[4] repeatedly divides clusters based on the largest eigenvalue and corresponding eigenvector of the modularity matrix.

Main Contributions

Two heuristics:

- LP relaxation and Distance-based Rounding Algorithm;
- Quadratic Programming and Randomized Rounding Algorithm.

One potential method ratio analysis:

- Similarity with Min-Disagree problem (4-approx) in LP formulation.

Pitfalls

- No ratio analysis over the LP rounding or randomized rounding for SDP;
- Significant huge resource requirement due to $\Theta(n^3)$ constraints in LP and $\Theta(n^2)$ variables in the vector programming; $\Longleftrightarrow$ Huge time complexity and computation overhead;
- Performance of LP rounding relies on the selection of center vertex.

Linear Programming Algorithm

- IP Formulation and LP relaxation;
- Distance-based Rounding;

IP formulation

Integer Program

Maximize

$$\frac{1}{2m} \cdot \sum_{u,v} (a_{u,v} - \frac{d_u d_v}{2m}) \cdot (1 - x_{u,v})$$

Subject to

$$x_{u,w} \leq x_{u,v} + x_{v,w} \qquad \forall u, v, w \in V$$

$$x_{u,v} \in \{0, 1\} \qquad \forall u, v \in V$$

Let

$$m_{u,v} = \frac{a_{u,v}}{2m} - \frac{d_u d_v}{4m^2}$$

LP formulation

Linear Program

Maximize

$$\sum_{u,v} m_{u,v} \cdot (1 - x_{u,v})$$

Subject to

$$x_{u,w} \leq x_{u,v} + x_{v,w} \qquad \forall u, v, w \in V$$

$$x_{u,v} \geq 0 \qquad \forall u, v \in V$$

Use CPlex to solve it $\Longrightarrow \Theta(n^3) constraints$

Distance-based rounding

Algorithm 1

$dist(u, v) \leftarrow x_{u,v}$ for LP solution X;

$S \leftarrow V$;

while $S \neq \emptyset$ **do**

  Select $u \in S$; $\triangleright$ randomly select

  $T_u \leftarrow \{v | dist(u, v) \leq 1/2\}$

  if average $dist(u, v) < 1/4$ for all $v \in \{T_u \setminus \{u\}\}$ **then**

    Make $C = T_u$ a cluster;

  else

    Make $C = \{u\}$ a singleton cluster

$S \leftarrow S \setminus C$;

Refine the result using local-search algorithm.

How good can this heuristic be?

Analysis

Definition

Min-Disagree problem formulated by [3]:

- Given a **complete** graph where all edges are labeled as respectively '+' or '-' to indicate the similarity or dis-similarity of vertex pair;
- partition the graph into clusters such that the number of errors ('-' edges within clusters and '+' edges between clusters) are minimized.

Analysis(Cont')

Min-Disagree LP

Minimize $\sum_{(u,v)\in E_+} x_{u,v} + \sum_{(u,v)\in E_-} (1 - x_{u,v})$

$\iff$ $|E_+| - \sum_{(u,v)\in E} \mu_{u,v}(1 - x_{u,v})$

Subject to

$$x_{u,w} \leq x_{u,v} + x_{v,w} \qquad \forall u, v, w \in V$$

$$x_{u,v} \geq 0 \qquad \forall u, v \in V$$

where $\mu_{u,v} = 1$ if (u, v) is '$+$' edge, otherwise 0.

Analysis(Cont')

Further results:

- if define

$$\mu_{u,v} = m_{u,v} = \frac{a_{u,v}}{2m} - \frac{d_u d_v}{4m^2}$$

  Mis-Degree formulation on **complete** graph is similar to the IP formulation of modularity maximization.

- Mis-Degree problem has a 4-approximation rounding algorithm;
- Due to existence of $|E_+|$, it is hard to get a same approximation algorithm for modularity maximization.

Vector Programming Algorithm

Kernel:

- Formulate the problem as Quadratic Program;
- Relax to vector program (Semi-definite programming);
- Use randomized cutting hyperplane to round the SDP solution.

Quadratic Programming Formulation

Considering **partitioning the graph into two communities** $(S, \bar{S})$ **of maximum modularity**, let $y_v = \pm 1$ indicate that vertex v belongs (or not) to S. Therefore, the formulation is:

Quadratic Program

Maximize

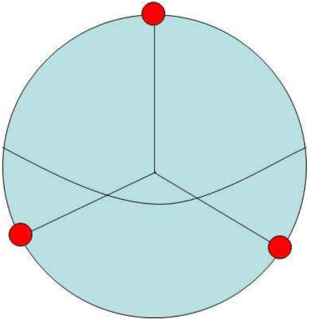
$$\frac{1}{4m} \sum_{u,v \in V} m_{u,v}(1 + y_u y_v)$$

Subject to

$$y_v^2 = 1 \text{ for all } v$$

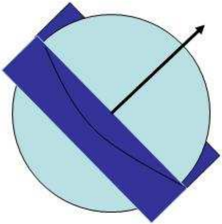
Semi-definite Relaxation

Key idea: relax $y = \pm 1$ to n-dimensional vector $\overrightarrow{y}$ with $\| y \| = 1$.



The product of $y_u y_v$ is corresponding to inner product of $\overrightarrow{y_u} \bullet \overrightarrow{y_v} = \cos\theta$

Randomized Rounding



- randomly select a n-dimension vector $\overrightarrow{s}$, where each component is following independent $\mathcal{N}(0,1)$ Gaussian.
- $S = \{v | \overrightarrow{y_v} \bullet \overrightarrow{s} \geq 0\}$
- $\bar{S} = \{v | \overrightarrow{y_v} \bullet \overrightarrow{s} < 0\}$

Algorithm

Algorithm 2

Hierarchical Clustering:

- use Semi-definite programming find a near-optimal division of a larger cluster $\Longleftrightarrow$ locally optimal;
- repeat the division until no further partition will increase the modularity;
- do local search post-processing to refine the solution.

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