

Course project

«Optimization approaches to community detection»

Marina Danilova, Alexander Podkopaev, Nikita Puchkin,
Igor Silin

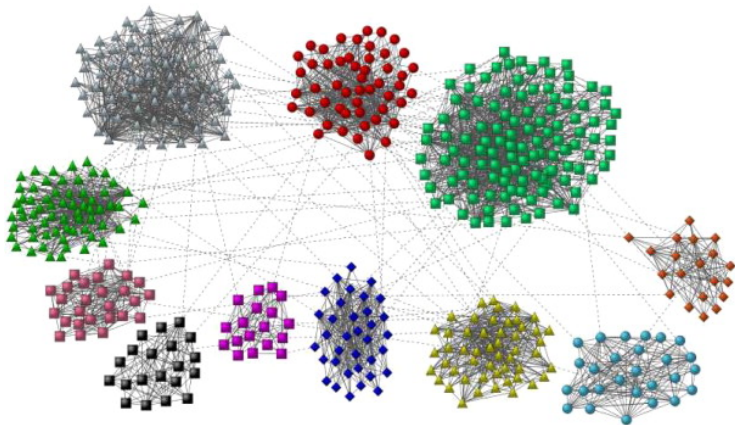
SKOLKOVO INSTITUTE OF SCIENCE AND TECHNOLOGY

December 16, 2016

Plan

- 1 Introduction to community detection
- 2 Algorithms
 - Modularity-based method
 - Spectral method
 - Semidefinite relaxation method
 - Natural conjugate gradients method
- 3 Experimental results

Example



The goal of community detection is to find **partition** of nodes into **non-overlapping** clusters.

Notations

Graph

- **Undirected unweighted graphs without loops** with n nodes and m edges.
- The nodes are enumerated as $\{1, \dots, n\}$.
- Graph is given by its $n \times n$ adjacency matrix A .
- Degree of the node i is d_i .

Clusters

- The number of clusters is k .
- The clusters are denoted as $\mathcal{C}_1, \dots, \mathcal{C}_k$.
- Cluster sizes are $|\mathcal{C}_1|, \dots, |\mathcal{C}_k|$.
- Labeling z : $z(i)$ is the cluster containing node i , i.e. $i \in \mathcal{C}_{z(i)}$.

Modularity-based method

Modularity

- Fraction of edges which lie within communities:

$$\frac{1}{2m} \sum_{i,j=1}^n a_{ij} \cdot \mathbb{1}\{z(i) = z(j)\}.$$

- Expected fraction of edges which lie within communities (for some probabilistic model):

$$\sum_{i,j=1}^n \frac{d_i}{2m} \frac{d_j}{2m} \cdot \mathbb{1}\{z(i) = z(j)\}.$$

- Modularity** is the difference between two previous fractions:

$$Q(z) = \frac{1}{2m} \sum_{i,j=1}^n \left(a_{ij} - \frac{d_i \cdot d_j}{2m} \right) \cdot \mathbb{1}\{z(i) = z(j)\}.$$

Modularity-based method

Formulating an optimization problem

$$\begin{aligned} & \text{maximize } Q \\ & \text{s.t. all possible labelings } z \end{aligned}$$

Greedy algorithm

1. Initially every node forms its own cluster: $\mathcal{C}_i = \{i\}$ and $Q = 0$.
2. Iteratively:
 - choose two current clusters, joining of which gives maximal gain ΔQ of modularity.
 - unite these two current clusters into one and recalculate $Q := Q + \Delta Q$.
3. Pick the clustering with maximal Q from partitions that we had during the iterations.

Spectral method

Measuring sizes of clusters

Consider the following two ways of measuring size of clusters:

- $|\mathcal{C}_i| = \{\text{number of vertices in } \mathcal{C}_i\}$
- $vol(\mathcal{C}_i) = \sum_{i \in \mathcal{C}_i} d_i$

MinCut

Define $W(\mathcal{C}_p, \mathcal{C}_q) := \sum_{i \in \mathcal{C}_p, j \in \mathcal{C}_q} a_{ij}$. Then MinCut problem is:

$$cut(\mathcal{C}_1, \dots, \mathcal{C}_k) = \frac{1}{2} \sum_{i=1}^k W(\mathcal{C}_i, \overline{\mathcal{C}_i}) \rightarrow \min_{\mathcal{C}_1, \dots, \mathcal{C}_k}$$

Spectral method

RatioCut and Normalized Cut

The MinCut solution separates one individual vertex from the rest. The following objectives are considered:

$$RatioCut(C_1, \dots, C_k) = \sum_{i=1}^k \frac{cut(C_i, \bar{C}_i)}{|C_i|} \rightarrow \min_{C_1, \dots, C_k}$$

$$NormCut(C_1, \dots, C_k) = \sum_{i=1}^k \frac{cut(C_i, \bar{C}_i)}{vol(C_i)} \rightarrow \min_{C_1, \dots, C_k}$$

Balancing conditions lead to NP-hard problem. Spectral clustering is a way to solve relaxed versions of those problems

Spectral method

Types of Laplacians

- Unnormalized Laplacian: $L = D - A$
- Symmetric Laplacian: $L_{sym} = D^{-\frac{1}{2}} L D^{-\frac{1}{2}} = I - D^{-\frac{1}{2}} A D^{-\frac{1}{2}}$
- Random walk Laplacian: $L_{rw} = D^{-1} L = I - D^{-1} A$

Idea

- Solving relaxed problem is equivalent to considering eigenvectors corresponding to k smallest eigenvalues of Laplacian that describe cluster properties of given graph

Semidefinite relaxation method

Clustering matrix

- Clustering matrix X of size $n \times n$ with $x_{ij} = \mathbb{1}\{z(i) = z(j)\}$.
- Space of all matrices with such structure is \mathcal{X} .

Formulating an optimization problem

Likelihood for special case of stochastic block model is

$$\mathcal{L}(X) = \text{trace}(AX).$$

Maximum likelihood method:

$$\begin{aligned} & \text{maximize } \mathcal{L}(X) \\ & \text{s.t. } X \in \mathcal{X} \end{aligned}$$

NP-hard combinatorial optimization problem \Rightarrow relaxations!

Semidefinite relaxation method

Semidefinite relaxation

We just relax $X \in \mathcal{X}$ and get semidefinite program:

$$\text{maximize } \text{trace}(AX)$$

s.t. X is positive semi-definite,

$$X \geq 0,$$

$$\text{diagonal}(X) = e,$$

$$Xe = \frac{n}{k}e,$$

where $e = (1, \dots, 1)^T$.

This problem can be solved with SDP solvers implemented in cvx.

Natural conjugate gradients method

- Model parametrized by

$$z(i) \sim \text{Poly}(\pi), \quad i = \overline{1, n}$$

$P = \|p_{ij}\|_{i,j=\overline{1,k}}$ - probabilities of inter-cluster edges occurrence

- Bayesian approach:

$$\pi \sim \text{Dirichlet}(\alpha)$$

$$p_{ii} \sim \text{Beta}(\beta), \quad i = \overline{1, k}$$

$$p_{ij} \ll 1, \quad \forall i \neq j$$

- $p(z, \pi, P|A)$ - true posterior with observed adjacency matrix A
- \mathcal{Q} - family of feasible distributions

Natural conjugate gradients method

Formulating an optimization problem

$$\mathcal{L}(q) \equiv -\text{KL}(q \| p(Z, \pi, P|A)) \longrightarrow \max_{q \in \mathcal{Q}}$$

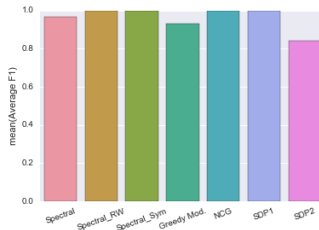
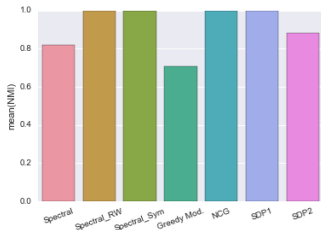
- The problem can be reduced to unconstrained optimization:

$$\mathcal{L} = \mathcal{L}(\theta) \longrightarrow \max, \quad \theta - n \times (k - 1) \text{ matrix}$$

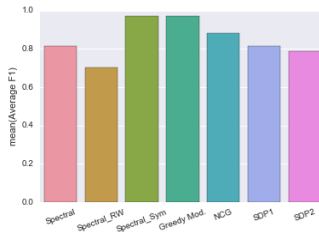
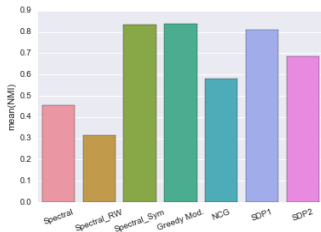
- Use conjugate gradients method in a statistical manifold
- Metrics is defined by a matrix

$$\mathcal{I}(\theta) - \text{Fischer information}$$

Artificial graph:



Real-world graph:



Thanks for your attention!