Semidefinite relaxations of the clustering program and first-order methods for their solution

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Agenda

Present a semidefinite relaxation for the graph clustering problem based on decomposition of graph into densest union of disjoint subgraphs.

Give a probabilistic model for “clusterable” data and graphs, and theoretical recovery guarantees.

Propose an ADMM algorithm for solving this relaxation.

Open problems.

Joint with Aleksis Pirinen, Lund University.
Clustering: partition data so that items in each cluster are similar to each other and items not in the same cluster are dissimilar.

Fundamental problem in statistics and machine learning:
- pattern recognition, computational biology, image processing/computer vision, network analysis.

No consensus on what constitutes a good clustering; depends heavily on application.

Intractable: usually modeled as some NP-hard problem (e.g. clique, normalized cut, k-means).
A sanity check

Clustering seems to be a very difficult/ill-posed problem.

Many heuristics seem to work well in practice.

**Question:** can we show that we can cluster “clusterable” data? How do we model clusterable data?
Graph clustering

**Similarity Graph:** represent data set as a graph

- items = nodes
- edges indicate similarity

Cluster the data set by dividing the graph into dense subgraphs.

Dense = large average degree
The Weighted Similarity Graph

Given data and affinity function $f$ indicating similarity between any two items.

Can model the data as *weighted similarity graph* $G_S = (V, E, W)$ as follows:

- Each item is represented by a node in $V$.
- We add an edge between each pair of two nodes $i, j$ with edge weight $w_{ij} = f(i, j)$.
- $w_{ij}$ is large if $i$ and $j$ are highly similar.
Example: Communities in Social Networks

- Nodes = users
- Edges = “friendship”.
- Densely connected groups = communities
Suppose each data point in the $i$th cluster $C_i$ is placed uniformly at random in a ball centered at $c_i \in \mathbb{R}^d$.

Distance within clusters will be small compared to the distance between clusters if centers are well-separated.

Choose $w_{ij} = \exp(-\|x^i - x^j\|^2)$. 

\[ Example: Clusters Euclidean data \]
Example: Clustered Euclidean data

Suppose each data point in the \(i\)th cluster \(C_i\) is placed uniformly at random in a ball centered at \(c_i \in \mathbb{R}^d\).

Distance within clusters will be small compared to the distance between clusters if centers are well-separated.

Choose \(w_{ij} = \exp(-\|x^i - x^j\|^2)\).
The Densest $k$-Disjoint Clique Problem

To cluster the data we want to partition the graph into cliques with heavy support.

A $k$-disjoint-clique subgraph of a graph $G$ is a subgraph of $G$ induced by $k$ disjoint cliques.

**Densest $k$-disjoint-clique problem (KDC):** find a $k$-disjoint-clique subgraph such that the sum of the densities of the $k$ complete subgraphs induced by the cliques is maximized.

**Density of complete subgraph induced by $C$:**

$$d(C) = \frac{1}{|C|} \sum_{i \in C} \sum_{j \in C} w_{ij} = \frac{v^T W v}{v^T v}$$

where $v$ is the characteristic vector of $C$. 
Lifting procedure for KDC

Let \( \{C_1, \ldots, C_k\} \) define a \( k \)-disjoint-clique subgraph with characteristic vectors \( \{v_1, v_2, \ldots, v_k\} \)

Lift the \( k \) characteristic vectors \( \{v_1, v_2, \ldots, v_k\} \) to the rank-\( k \) matrix variable \( X \):

\[
X = \sum_{i=1}^{k} \frac{v_i v_i^T}{\|v_i\|^2} = \sum_{i=1}^{k} \frac{v_i v_i^T}{|C_i|}
\]

Want to find \( X \) that maximizes

\[
\text{Tr}(WX) = \sum_{i=1}^{k} \frac{v_i^T W v_i}{\|v_i\|^2} = \sum_{i=1}^{k} d(C_i)
\]
Lifted solutions

Lifted solution $\mathbf{X}$ must satisfy:

- Inlier rows sum to 1. Outlier rows equal 0: $\mathbf{Xe} \leq \mathbf{e}$
- $\mathbf{X}$ is symmetric doubly nonnegative: $\mathbf{X} \succeq \mathbf{0}$, $\mathbf{X} \preceq \mathbf{0}$
- $\text{rank}(\mathbf{X}) = \text{Tr}(\mathbf{X}) = k$
- plus other combinatorial constraints
Ignoring rank constraint and relaxing combinatorial constraints on $X$ gives the semidefinite program:

$$\begin{align*}
\text{max} \quad & \text{Tr}(WX) \\
\text{st} \quad & X e \leq e \\
& \text{Tr}(X) = k \\
& X \geq 0, \quad X \succeq 0.
\end{align*}$$

**Question:** When does the optimal solution of this relaxation recover underlying cluster structure in similarity graph?
The Stochastic Block Model

**Stochastic Block Model (SBM):** generate random graph containing \( k \) clusters of size \( r \), where edges within-clusters are added with probability \( p \) and edges between-clusters are added with probability \( q < p \).

Chen/Xu (2014): characterize when graphs sampled from the SBM are easy to cluster (have polynomial-time algorithm), hard to cluster (via max likelihood), and impossible to cluster. In particular, \( n \)-node graph from SBM is easy to cluster if

\[
\frac{(p - q)^2}{q(1 - q)} = \Omega \left( \frac{n}{r^2} \right) .
\]

Many other papers establish similar results for different classes of algorithms, e.g., spectral clustering, convex/semidefinite relaxation, etc., as well as variants of the SBM with unbalanced clusters, outliers, heterogeneous edge probabilities, etc.
The Planted cluster model

Randomly generate weights $W \in [0, 1]^{n \times n}$ according to the following model:

- Start with clusters $C_1, \ldots, C_k$ of sizes $r_1, \ldots, r_k$. plus outlier set $C_{k+1}$ of size $r_{k+1}$.

- Sample entries of $W(C_i, C_i)$ i.i.d. from probability distribution $\Omega_1$ with mean $\alpha(n)$ and variance $\sigma_1^2(n)$.

- Sample remaining entries of $W$ i.i.d. from distribution $\Omega_2$ with mean $\beta(n) < \alpha(n)$ and variance $\sigma_2^2(n)$.

**Question:** under what conditions on $\alpha, \beta, \sigma_1, \sigma_2, r, n, k$ do we have perfect recovery of the clusters $C_1, \ldots, C_k$?
Suppose $W \in \Sigma^n$ is sampled from the planted cluster model.

Let $X^* = \sum_{i=1}^k \frac{v_i v_i^T}{r_i}$ denote the cluster matrix corresponding to the planted clusters $C_1, \ldots, C_k$.

Let $\hat{r} = \min_{i=1,\ldots,k} r_i$ and $\tilde{r} = \max_{i=1,\ldots,k} r_i$.

Let $\tilde{\sigma}^2 := \max\{\sigma_1^2, \sigma_2^2\}$. 
Guaranteed Recovery: Phase Transition

There exists constants $c_1, \ldots, c_5 > 0$ (independent of $\alpha, \beta, \hat{r}, n$) such that if

1. the gap assumption

$$\alpha - \beta \geq c_5 \max \left\{ \sqrt{\frac{\bar{\sigma}^2 \log n}{\hat{r}}}, \frac{\log n}{\hat{r}} \right\}$$

is satisfied, and

2. $\hat{r}$ satisfies

$$(\alpha - \beta)\hat{r} \geq c_1 \max \left\{ \sigma_2 \sqrt{n}, \sqrt{\log n} \right\} + c_2 \max \left\{ \sigma_1 \sqrt{\hat{r}}, \sqrt{\log n} \right\} + c_3 \left( \max \left\{ \frac{\sigma_2^2}{\hat{r}}, \frac{\log n}{\hat{r}} \right\} kr_{k+1} \right)^{1/2} + c_4 \beta r_{k+1}$$

then $\{C_1, \ldots, C_k\}$ is the unique densest $k$-disjoint-clique subgraph and $X^*$ is the unique optimal solution of the SDP relaxation with high probability.
This suggests that we can recover the planted clusters w.h.p. provided that

\[
\frac{(\alpha - \beta)^2}{\tilde{\sigma}^2} = \Omega \left( \frac{n}{\hat{r}^2} \right).
\]

The left-hand side acts as a signal-to-noise ratio: ratio of difference between expected edge weights to noise variance.

This agrees with/generalizes the easy regime for cluster recovery proposed by Chen and Xu (2014), and Jalali et al. (2015).

The relaxation is mostly parameter free: SDP needs number of clusters \( k \) but doesn’t need estimate of cluster sizes \( r_i \), gap statistic \( \alpha - \beta \), etc., seen in similar theoretical guarantees.
Suppose $\Omega_1$ and $\Omega_2$ are Bernoulli distributions with probability of adding an edge $p$ and $q$ respectively ($p > q$) with no outliers ($r_{k+1} = 0$).

**Dense case:** $p, q$ constant (independent of $n$).
Have exact recovery w.h.p. if $\hat{r} \geq \hat{c}\sqrt{n}$ for some scalar $\hat{c}$ (depending on $p, q$).

**Sparse case:** $p$ constant, $q \leq \frac{\log n}{n}$.
Have exact recovery w.h.p. if $\hat{r} \geq \tilde{c}\log n$ for some constant $\tilde{c}$.
Sensitivity to outliers

SBM with $k = 1$ specializes to the planted clique model. (Graph consists of a single complete subgraph obscured by noise).

Theorem suggests exact recovery with $\hat{r} = \Omega(r_{k+1}) = \Omega(n)$.

This far exceeds the standard planted clique recovery guarantee of $\hat{r} = \Omega(\sqrt{n})$ (in dense case).

Unfortunately this bound is tight.

- Expected value of $X^*$ is $p\hat{r}$.

- Expected value of $\frac{1}{n} \text{Tr}(W_{ee^T}) = \Omega(qn)$. Therefore, $X^*$ is suboptimal unless

  \[ \hat{r} = \Omega \left( \frac{p}{q} n \right). \]
Sensitivity to outliers (2)

\[ n = 10000 \]

\[ \hat{r} = 1200 = 12\sqrt{n}. \]

\[ \text{Tr}(WX^*) = 1200 \]

\[ < \frac{1}{n} \text{Tr}(\text{Wee}^T) \approx 1375 \]
Proof Outline

Can construct a choice of dual variables using KKT conditions.

Have a dual certificate when \( W = E[W] \).

Use concentration inequalities to show that this choice of dual variables is feasible w.h.p. when gap assumption and \( \hat{r} \) bound are met.

- Establish nonnegativity using Bernstein inequality.
- Establish semidefiniteness using the Matrix Bernstein Inequality (Bandeira and van Handel 2016).
Clustering SDP has $n \times n$ semidefinite variable and $m = O(n^2)$ (in)equality constraints.

Can be (approximately) solved in polynomial-time using interior point methods.

Costs $O(m^3) = O(n^6)$ flops per Newton iteration.

- Prohibitively expensive for large graphs/data.
Alternating Direction Method of Multipliers

Let $\Xi := \{ X \in \Sigma^V : X e \leq e, \ X \geq 0 \}.$ Let $\Omega := \{ X \in \Sigma^V : \text{Tr}(X) = k, \ X \in \Sigma^V_+ \}.$

Can rewrite Cluster SDP as:

$$\max_{X, Y} \{ \text{Tr}(W Y) : X - Y = 0, \ X \in \Xi, \ Y \in \Omega \}.$$ 

Augmented Lagrangian is

$$L_\rho(X, Y, U) = \text{Tr}(W Y) - \text{Tr}(U(X - Y)) + \frac{\rho}{2} \| X - Y \|^2_F.$$ 

Solve using ADMM: update iterate $(X^k, Y^k, U^k)$ by

$$Y^{k+1} = \arg \min_{Y \in \Omega} L_\rho(X^k, Y, U^k)$$

$$X^{k+1} = \arg \min_{X \in \Xi} L_\rho(X, Y^{k+1}, U^k)$$

$$U^{k+1} = U^k - \rho(X^{k+1} - Y^{k+1}).$$
Updating $Y$

$Y^{k+1}$ is a minimizer of the subproblem

$$\min_{Y \in \Omega} \frac{1}{2} \left\| Y - \left( X^k - \frac{1}{\rho} (W + U^k) \right) \right\|_F^2.$$

Let $X^k - \frac{1}{\rho} (W + U^k)$ have eigenvalue decomposition $V \text{Diag}(v^k) V^T$.

Then $Y^{k+1} = V \text{Diag}(y^*) V^T$ where $y^*$ is the projection of $v^k$ onto the simplex

$$\left\{ y : e^T y = k, \ y \geq 0 \right\}.$$
Updating $X$

$X^{k+1}$ is a minimizer of the subproblem

$$\min_{X \in \Xi} \frac{1}{2} \left\| X - \left( Y^{k+1} + \frac{1}{\rho} U^k \right) \right\|_F^2.$$

Has dual problem

$$\min_{z \geq 0} \frac{1}{2} \left\| \left[ \left( Y^{k+1} + \frac{U^k}{\rho} \right) - \frac{ze^T + ez^T}{2} \right] + z^T e \right\|_F^2 + z^T e$$

can be efficiently solved for $z^*$ using the spectral projected gradient method of Birgin et al. 2000.

Update $X$ by

$$X^{k+1} = \left[ \left( Y^{k+1} + \frac{1}{\rho} U^k \right) - \frac{z^* e^T + e(z^*)^T}{2} \right]_+ ;$$

here $([Z]_+)^{ij} = \max\{0, z_{ij}\}$. 
Numerical results

Add within-cluster edges independently with prob $p = 0.75$ and between-cluster edges with prob $q = 0.25$.

Fix $k = 4$ equal sized clusters so that $n = k \hat{r}$; let $\hat{r}$ vary from 10 to 40.

Solve with SDPT3 (using CVX) and our ADMM algorithm.
Numerical results (2)

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<th>SDPT3</th>
<th>ADMM</th>
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Future work: low-rank factorization

Have an alternate nonconvex relaxation:

$$\max_{Y \in \mathbb{R}^{n \times k}} \left\{ \text{Tr}(Y^T W Y) : YY^T e \leq e, \text{Tr}(YY^T) = \|Y\|_F^2 = k, Y \geq 0 \right\}$$

Burer and Monteiro 2003, 2005 propose this approach and related augmented Lagrangian method.

Wainwright and Chen 2016 analyze gradient methods for similar low-rank factored problems.

Evaluation of the augmented Lagrangian and its gradient cost $O(n^2k)$ flops.

Much further work is needed to show that overall run-time is competitive with ADMM and characterize recovery properties.
**Future work: heterogeneous distributions**

**Conjecture:** can strengthen recovery guarantee to following case:

- If \( u, v \) cluster \( C_i \) then \( E[w_{uv}] = \alpha_i \).
- If \( u \in C_i, v \in C_j, i \neq j \) then \( E[w_{uv}] = \beta_{ij} \).
- **Weak assortativity:** Replace \( \alpha - \beta \) with

\[
\min_i \left( \alpha_i - \max_j \beta_{ij} \right)
\]
**Future work: heterogeneous distributions**

**Conjecture:** can strengthen recovery guarantee to following case:

- If $u, v$ cluster $C_i$ then $E[w_{uv}] = \alpha_i$.

- If $u \in C_i, v \in C_j, i \neq j$ then $E[w_{uv}] = \beta_{ij}$.

- **Weak assortativity:** Replace $\alpha - \beta$ with

$$\min_i \left( \alpha_i - \max_j \beta_{ij} \right)$$
Matlab implementations available from bpames.people.ua.edu/software

Preprint: arxiv.org/abs/1603.05296

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