

GRAPH CLUSTERING AND THE NUCLEAR WASSERSTEIN METRIC.

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ABSTRACT. We study the problem of learning the cluster structure of a random graph \mathcal{G} from an independent sample. We propose a Wasserstein robust formulation of this optimization problem and prove that it can be reformulated as a tractable convex optimization problem. We give theoretical exact recovery guarantees for this problem when the Wasserstein metric is induced by the nuclear norm and \mathcal{G} is distributed according to the stochastic block model. Finally we present our Julia implementation of the proposed algorithm and show its numerical performance on synthetic data.

1. INTRODUCTION

Let \mathcal{G} be a random graph with n vertices. By a deterministic summary of \mathcal{G} we mean a (deterministic) graph H^* which, on average, differs from \mathcal{G} by as few edges as possible. In this article we study the problem of finding deterministic summaries *from an independent sample* of \mathcal{G} of size N . More precisely we address the following problem:

Problem 1.1. *Given adjacency matrices B_1, \dots, B_N of an independent sample of \mathcal{G} find a symmetric matrix A^* in $\arg \min_A \mathbb{E}_{B \sim \mathcal{G}}[\|A - B\|_1]$.*

Special cases of this problem arise in cluster detection and in data summarization, both heavily studied in the literature (see Section 1.1 for details).

A possible approach to problem 1.1 is to use the samples to construct the empirical measure $\hat{\mu} := \sum_{i=1}^N \frac{1}{N} \delta_{B_i}$ as an approximation of the distribution of \mathcal{G} and to find a minimizer A of the resulting empirical risk

$$\mathbb{E}_{B \sim \mu}[\|A - B\|_1] = \frac{1}{N} \sum_{i=1}^N \|A - B_i\|_1.$$

This approach is consistent and will lead to an optimal solution as the sample size $N \rightarrow \infty$. However, when the sample size N is not sufficiently large (typically one has few samples of very large graphs) for $\hat{\mu}$ to be a good approximation for the distribution of \mathcal{G} this approach leads to overfitting. To mitigate this problem we propose a robust version of Problem 1.1. In the robust version one aims to minimize the worst-case risk when the distribution of B is allowed to vary in a ball $\mathcal{N}_\delta(\hat{\mu})$ of radius $\delta > 0$ centered at the empirical measure $\hat{\mu}$ in a suitable metric, leading to

2000 *Mathematics Subject Classification.* Primary 15A29 Secondary 15B52, 52A22.

Key words and phrases. Compressed sensing, truncated moment problems, Kostlan-Shub-Smale polynomials.

Problem 1.2. *Given adjacency matrices B_1, \dots, B_N of an independent sample of \mathcal{G} find a symmetric matrix \bar{A} which minimizes the robust worst-case risk*

$$R_\delta(A) := \left(\sup_{\nu \in \mathcal{N}_\delta(\hat{\mu})} \mathbb{E}_{B \sim \mathcal{G}} [\|A - B\|_1] \right).$$

The robust worst-case risk is obviously dependent on the chosen metric among probability distributions. In this article we will use the Wasserstein metric $W_{\|\bullet\|}$ induced by a norm $\|\bullet\|$ on the space K of symmetric matrices with entries in $[0, 1]$. More precisely, if ν_1, ν_2 are probability measures on K and $\Pi(\nu_1, \nu_2)$ is the set of random variables (Z_1, Z_2) taking values in $K \times K$ with $Z_i \sim \nu_i$ then the Wasserstein distance between ν_1 and ν_2 is given by

$$W_{\|\bullet\|}(\nu_1, \nu_2) := \inf_{(Z_1, Z_2) \in \Pi(\nu_1, \nu_2)} \mathbb{E}[\|Z_1 - Z_2\|].$$

The seminal work of Esfahani and Kuhn [23] shows that robust formulations defined using the Wasserstein metric often lead to tractable convex optimization problems. Our first result is that this is also true for Problem 1.2 when the Wasserstein metric is induced by any semidefinitely representable norm.

Theorem 1.3. *Let K be the set of $n \times n$ symmetric matrices with entries in $[0, 1]$, let $\|\bullet\|$ be a norm on K and let $\delta > 0$. Problem 1.2 is equivalent to:*

$$\min_{(A, s_1, \dots, s_N, \lambda) \in \mathcal{T}} \left(\lambda\delta + \frac{1}{N} \sum_{i=1}^N s_i \right)$$

where \mathcal{T} is the set of $(A, \vec{s}, \lambda) \in K \times \mathbb{R}^n \times \mathbb{R}$ satisfying the inequalities $\lambda \geq 0$ and $\eta_{E,i}(\lambda) \leq s_i$ as $i = 1, \dots, N$ and E ranges over the set of all $\{-1, 1\}$ -symmetric matrices, where

$$\eta_{E,i}(\lambda) := \sup_{Y \in K} (\langle E, A - Y \rangle - \lambda \|B_i - Y\|)$$

The reformulation in Theorem 1.3 transforms the problem into a finite-dimensional convex optimization problem which unfortunately contains an exponential number of constraints. To address this problem we introduce:

- (1) A more tractable simplification which agrees with the original problem whenever the optimal \bar{A} occurs at a matrix with entries in $\{0, 1\}$.
- (2) A relaxation of (1) which takes the form of a regularized empirical risk minimization problem.

leading to practical algorithms for graph summarization. More specifically, if $\mathcal{S}^{n \times n}$ denotes the space of real symmetric $n \times n$ matrices we prove the following

Theorem 1.4. *If A is a symmetric $\{0, 1\}$ -matrix and $\delta > 0$ then:*

- (1) *The following equality holds:*

$$R_\delta(A) = \min_{\mathcal{H}} \left(\lambda\delta + \frac{1}{N} \sum_{i=1}^N s_i + \frac{1}{N} \sum_{i=1}^N \|A - B_i\|_1 \right)$$

where \mathcal{H} is the set of $(\lambda, s_1, \dots, s_N, \Lambda, W) \in \mathbb{R} \times \mathbb{R}^N \times \mathcal{S}^{n \times n} \times \mathcal{S}^{n \times n}$ which satisfy the inequalities:

$$\begin{aligned} \|W\|_* &\leq \lambda \\ \Lambda &\geq 0 \\ 2A - 11^t - W + \Lambda &\geq 0 \\ \|\Lambda\|_1 &\leq s_i - \langle 2A - 11^t - W, B_i \rangle \text{ for } i = 1, \dots, N \end{aligned}$$

(2) The following inequality holds:

$$R_\delta(A) \leq \frac{1}{N} \sum_{i=1}^N \|A - B_i\|_1 + \delta \|2A - 11^t\|_*.$$

Moreover, if $\|\cdot\|$ is a semidefinitely representable function then both (1) and the minimization of the right hand side of (2) for $A \in K$ are semidefinite programming problems.

Solving the optimization problems in Theorem 1.4 leads to a new algorithm for estimating deterministic graph summaries which we call *Wasserstein robust graph summarization*. We carried out extensive numerical experiments applying this algorithm to a variety of graphs G distributed according to the stochastic block model and observed that the regularized problem with the Wasserstein metric induced by the spectral norm was able to recover the correct cluster structure using only very few samples outperforming all others. This leads us to propose the *Wasserstein robust nuclear norm summarization problem*, given by

$$(1) \quad \min_{A \in K} \left(\frac{1}{N} \sum_{i=1}^N \|A - B_i\|_1 + \delta \|2A - 11^t\|_* \right)$$

where the nuclear norm $\|B\|_*$ of a matrix B is the dual of the spectral norm and equals the sum of its singular values.

A central result of this article is an exact recovery guarantee for this algorithm. More precisely, we show that exact recovery occurs for suitable $\delta > 0$ with overwhelming probability on samples distributed according to the stochastic block model, explaining the good practical performance of Wasserstein nuclear norm summarization in cluster detection. In order to describe our exactness guarantee we need to establish notation for the parameters of the stochastic block model. Recall that a random graph \mathcal{G} has distribution given by the stochastic block model in n vertices if there is a partition of $[n]$ into disjoint subsets C_1, \dots, C_k , real numbers $0 \leq q < \frac{1}{2} < p_1, \dots, p_k \leq 1$ and edges are added independently with probability p_{ij} of joining vertices i, j given by

$$p_{ij} := \begin{cases} p_t, & \text{if } \{i, j\} \subseteq C_t \\ q, & \text{else.} \end{cases}$$

Such a random graph \mathcal{G} has a unique deterministic summary A^* obtained by putting edges only between vertices belonging to the same cluster.

Theorem 1.5. *Suppose B_1, \dots, B_N are independent and are distributed according to \mathcal{G} . If $\alpha = \min(|p_t - \frac{1}{2}|, |q - \frac{1}{2}|)$ and δ^* is the maximum of $a(\delta) := \frac{\delta(\alpha - \frac{\delta}{n})^2}{(1 + \frac{2\delta}{n})}$ in $[0, \alpha n]$ then the probability that A^* is not the unique minimizer of (1) is bounded above by*

$$\exp\left(-\frac{2N(n-1)^3(\alpha n - \delta^*)^2}{n}\right) + e^{-N(\delta^* a(\delta^*))} \prod_{i \neq j} \left(1 + (e^{-4a} \widetilde{p}_{ij} + \widetilde{q}_{ij})^{\frac{N}{2}}\right).$$

which decreases exponentially with the sample size N .

The key point of the proof of Theorem 1.5, discussed at length in Section 3, is that the subdifferential of the regularization term at A^* is sufficiently rich so as to contain enough transportation matrices. This gives a geometric explanation for why the nuclear norm is a good regularizer for graph summarization problems.

Finally we focus on the practical performance of the proposed algorithm. Solving the optimization problems appearing in Theorem 1.4 typically require solving large semidefinite programs which are beyond the capacity of standard off-the-shelf software even for relatively small graphs (of say 40 vertices with $N = 4$). One possible reason is that off-the-shelf solvers often use interior point methods, which are highly accurate but often do not scale well. A better alternative, especially well suited for Wasserstein robust nuclear norm summarization is to use first order numerical optimization methods such as the alternating direction method of multipliers (ADMM). In Section 4.3 we adapt the ADMM algorithm to our regularized problem and present our open source Julia implementation. This implementation can run the Wasserstein nuclear norm summarization algorithm in graphs of up to 10000 vertices and $N \leq 10$ on a common laptop.

1.1. Relation to previous work. Understanding structural properties of graphs is a problem of high interest since graphs appear naturally in many areas. The problem of finding communities in a graph is one of the most studied tasks in machine learning, with applications to Biology [7, 14, 29], social data understanding [16, 22, 25] and other general machine learning tasks such as natural language processing [15, 27]. One of the reasons of the importance of this problem is that it allows researchers to organize datasets into sets of similar observations, and then apply learning algorithms on each of the sets. Most theoretical results in the community detection problem occur in the context of generative random graph models. Of these the most studied is the stochastic block model [1] which is particularly important since in it communities are defined a priori and thus there is a formally specified underlying true cluster structure with which the output of algorithms can be compared.

There are three main approaches for the problem of community detection on a (single) graph:

- (1) Spectral clustering algorithms, widely used in the detection of sparse communities [5, 13, 20, 21].
- (2) SDP approaches based on the seminal work of Goemans and Williamson [18], [2, 19, 24].

- (3) Decompositions of the adjacency matrix of the graph into a matrix of low rank and a sparse (noise) matrix, using a convex relaxation based on the nuclear norm [8, 10, 9]. These methods have led to several convex optimization algorithms to find communities in graphs [4, 28, 12, 11, 26, 3].

The results in this article differ from previous work in two main accounts:

- (1) Our methods apply to the problem of learning from *several* samples while, to the best of our knowledge, the above algorithms must be applied to a single graph. Practitioners resort to several “graph combination” methods to transform datasets consisting of several samples into one. Our methods do not require this additional pre-processing step and are able to use the additional information contained in several samples to obtain more accurate recovery (see Section 4.3)
- (2) Formulating learning problems as Wasserstein robust optimization problems leads to regularization algorithms in a principled way. Even in the single-sample case this leads to improvements in performance when compared for instance with the sparse+low-rank approach (see Section 4.3).

1.2. Acknowledgments. We wish to thank Fabrice Gamboa, Mauricio Junca and Thierry Klein for useful conversations during the completion of this project. D. De Roux was partially supported by a grant from Facultad de Ciencias, Universidad de los Andes and by CAOBA. M. Velasco was partially supported by research funds from Universidad de los Andes.

2. ROBUST LEARNING OF DETERMINISTIC SUMMARIES

Let $[n] := \{1, 2, \dots, n\}$. By a graph G on $[n]$ we mean a finite loopless undirected graph with vertex set $[n]$. The adjacency matrix of such a graph is a symmetric $n \times n$ matrix with entries in $\{0, 1\}$ and ones in positions (i, j) whenever vertices i and j are adjacent. Let \mathcal{A}_n be the set of adjacency matrices of graphs on $[n]$ (i.e. $\{0, 1\}$ -matrices of size $n \times n$ which are symmetric and have zeroes in the diagonal). Throughout the article we will use graphs and their adjacency matrices interchangeably. By a random graph \mathcal{G} on $[n]$ we mean a random variable B taking values in \mathcal{A}_n . For a matrix B we let $\|B\|_p$ to be the p -th root of the sum of the p -th powers of its entries. We denote by $\langle A, B \rangle := \text{Tr}(AB)$ the Frobenius inner product on symmetric matrices.

Definition 2.1. *A deterministic summary of a random graph \mathcal{G} on $[n]$ is a graph A^* with $A^* \in \arg \min_{A \in \mathcal{A}_n} \mathbb{E}[\|A - \mathcal{G}\|_1]$.*

The deterministic summary A^* is a graph which, on average, differs from \mathcal{G} by the smallest possible number of edges. If the distribution of \mathcal{G} is known it is easy to find a deterministic summary (which is often unique). More precisely,

Lemma 2.2. *If $\mathbb{P}\{(i, j) \in \mathcal{G}\} \neq \frac{1}{2}$ for all $i, j \in [n]$ then the unique deterministic summary of \mathcal{G} is given by A^* with*

$$A_{ij}^* = \begin{cases} 1, & \text{if } \mathbb{P}\{(i, j) \in \mathcal{G}\} > \mathbb{P}\{(i, j) \notin \mathcal{G}\} \\ 0, & \text{if } \mathbb{P}\{(i, j) \in \mathcal{G}\} < \mathbb{P}\{(i, j) \notin \mathcal{G}\} \end{cases}$$

Proof. If $A \in \mathcal{A}_n$ then the term coming from entry (i, j) in $\mathbb{E}[\|A - \mathcal{G}\|_1]$ is given by $|A_{ij} - 1|p + |A_{ij}|q$ where p (resp q) is the probability that (i, j) is (resp. is not) an edge of \mathcal{G} . This quantity is greater than $\min(p, q)$ and equality is achieved, for all i, j when $A = A^*$. \square

Motivated by the previous Lemma we define a cluster structure on a random graph.

Definition 2.3. *A random graph \mathcal{G} has a cluster structure or a community structure if it has a unique deterministic summary A^* and the corresponding graph is a disjoint union of cliques. We call these cliques the clusters of \mathcal{G} .*

The main problem that we address in this article is that of *learning* deterministic summaries (and in particular the problem of learning cluster structures on random graphs who have them). By this we mean that our only knowledge about the distribution of the random graph \mathcal{G} is encoded in an independent sample B_1, \dots, B_N of adjacency matrices with the same distribution as \mathcal{G} , leading to Problem 1.1 in the Introduction.

Given the sample, define the empirical measure $\hat{\mu} := \frac{1}{N} \sum_{j=1}^N \delta_{B_j}$ as a sum of Dirac delta measures at the sample points. As the number of sample points increases the measure $\hat{\mu}$ converges to the distribution of \mathcal{G} [17] and it is therefore reasonable to try to minimize the objective function in Problem 1.1 with respect to the measure $\hat{\mu}$ instead of \mathcal{G} , that is by finding a minimizer of the empirical risk

$$\bar{A} \in \arg \min_{A \in K} \mathbb{E}_{Z \sim \hat{\mu}} [\|A - Z\|]$$

Arguing as in Lemma 2.2 it is immediate that a (generally unique) minimizer \bar{A} is given by counting edge frequencies, that is

$$\bar{A}_{ij} := \begin{cases} 1, & \text{if } |\{t : B_{ij}^{(t)} = 1\}| > |\{t : B_{ij}^{(t)} = 0\}| \\ 0, & \text{if } |\{t : B_{ij}^{(t)} = 1\}| < |\{t : B_{ij}^{(t)} = 0\}| \end{cases}$$

The empirical risk minimization approach has lots of advantages, it is easy to implement, scales very well and is guaranteed to be consistent (in the sense that $\bar{A}_{ij} \rightarrow \bar{A}$ as the number of samples $N \rightarrow \infty$). However it also suffers from some potential drawbacks:

- (1) If the sample size N is small then the empirical measure $\hat{\mu}$ could be very far from the distribution of \mathcal{G} .
- (2) The estimation of \bar{A} is done independently edge by edge and in particular it does not use any global information, for instance the existence of a cluster structure as part of the estimation process.

To mitigate these problems we will use a robust formulation. To this end let $\|\bullet\|$ be a norm in the space of symmetric $n \times n$ matrices and let $W_{\|\bullet\|}$ be the Wasserstein distance induced by a given norm $\|\bullet\|$ on K . For a real number $\delta \geq 0$ let $\mathcal{N}_\delta(\hat{\mu})$ be the (closed) ball of radius δ centered at $\hat{\mu}$. We would like to solve the following

Problem. Given adjacency matrices B_1, \dots, B_N of an independent sample of \mathcal{G} find a symmetric matrix \bar{A} which minimizes the robust worst-case risk

$$R_\delta(A) := \left(\sup_{\nu \in \mathcal{N}_\delta(\hat{\mu})} \mathbb{E}_{B \sim \mathcal{G}} [\|A - B\|_1] \right).$$

Our first result reformulates the robust optimization above as a finite convex optimization problem by closely following the ideas of Esfahani and Kuhn. The proof is included for the reader's benefit.

Proof of Theorem 1.3. Let \mathcal{M} be the set of probability measures in $K \times K$ whose marginal distribution in the first component is given by the empirical measure $\hat{\mu}$. Every such measure is of the form

$$\nu = \sum_{i=1}^N \frac{1}{N} \delta_{B_i} \otimes \mathbb{Q}_i$$

where \mathbb{Q}_i is a probability measure on K . Conditioning on the value of X it is immediate that these measures act on functions on two sets of variables corresponding to each copy of K via the formula

$$\int_{K \times K} f(x, y) d\nu = \sum_{i=1}^N \frac{1}{N} \int_K f(B_i, y) d\mathbb{Q}_i(y).$$

The distribution of a random variable $Y \in K$ lies in the Wasserstein ball $\mathcal{N}_\delta(\hat{\mu})$ iff there exists a random vector $(X, Y) \in K \times K$ with distribution $\nu \in \mathcal{M}$ which satisfies $\int_{K \times K} \|X - Y\| d\nu \leq \delta$. This description will allow us to optimize over $\mathcal{N}_\delta(\hat{\mu})$. If $A \in K$ then the following equalities hold:

$$R_\delta(A) = \sup_{\nu \in \mathcal{M}} \left(\int_{K \times K} \|A - Y\|_1 d\nu : \int_{K \times K} \|X - Y\| d\nu \leq \delta \right)$$

which can be written as

$$\sup_{\nu \in \mathcal{M}} \inf_{\lambda \geq 0} \int_{K \times K} \|A - Y\|_1 d\nu + \lambda \left(\delta - \int_{K \times K} \|X - Y\| d\nu \right)$$

By strong duality for moment problems this quantity equals

$$\inf_{\lambda \geq 0} \sup_{\nu \in \mathcal{M}} \int_{K \times K} \|A - Y\|_1 d\nu + \lambda \left(\delta - \int_{K \times K} \|X - Y\| d\nu \right)$$

and conditioning on the value of X we compute the integrals obtaining

$$\inf_{\lambda \geq 0} \lambda \delta + \frac{1}{N} \sup_{\mathbb{Q}_1, \dots, \mathbb{Q}_N} \left(\int_K \|A - Y\|_1 - \lambda \|B_i - Y\| d\mathbb{Q}_i(Y) \right).$$

Since the integrals are maximized when the \mathbb{Q}_i are Dirac deltas at optima of their corresponding functions we conclude that this quantity equals

$$\inf_{\lambda \geq 0} \lambda \delta + \frac{1}{N} \sup_{Y \in K} (\|A - Y\|_1 - \lambda \|B_i - Y\|)$$

Next we move the supremum into the constraints obtaining

$$\inf_{(\lambda, s_1, \dots, s_n)} \left(\lambda \delta + \frac{1}{N} \sum_{i=1}^N s_i : \sup_{Y \in K} (\|A - Y\|_1 - \lambda \|B_i - Y\|) \leq s_i, \text{ for } i = 1, \dots, N \right).$$

Finally, if L denotes the set of symmetric matrices with entries in $\{-1, 1\}$ then the following equalities hold for every symmetric matrix B

$$\|B\|_1 = \sup_{H: \|H\|_\infty \leq 1} \langle B, H \rangle = \max_{E \in L} \langle B, E \rangle.$$

Defining the concave function

$$\eta_{E,i}(\lambda) := \sup_{Y \in K} (\langle E, A - Y \rangle - \lambda \|B_i - Y\|)$$

we therefore conclude that

$$R_\delta(A) = \inf_{(\lambda, s_1, \dots, s_n)} \left(\lambda \delta + \frac{1}{N} \sum_{i=1}^N s_i : \eta_{E,i}(\lambda) \leq s_i \text{ for all } E \in L \text{ and } i = 1, \dots, N \right).$$

Letting A vary in K we prove the Theorem. \square

Our second results gives a simplification of the previous problem which agrees with it when problem 1.2 has an optima which occurs at a matrix with entries in $\{0, 1\}$. The proof is similiar to the proof of 1.3.

Proof of Theorem 1.4. If the symmetric matrix A has entries in $\{0, 1\}$ and X, Y are matrices in K then the following equalities hold

$$\|A - Y\|_1 = \langle 2A - 11^t, A - Y \rangle = \|A - X\|_1 + \langle 2A - 11^t, X - Y \rangle$$

Now suppose (X, Y) is a random vector taking values in $K \times K$ with distribution ν in the set \mathcal{M} of the proof of Theorem 1.3. Taking expected values and suprema we see that

$$(2) \quad R_\delta(A) = \frac{1}{N} \sum_{i=1}^N \|A - B_i\|_1 + \sup_{\nu \in \mathcal{M}} \int_{K \times K} \langle 2A - 11^t, X - Y \rangle d\nu$$

Since $\langle 2A - 11^t, X - Y \rangle \leq \|2A - 11^t\|_* \|X - Y\|$ by definition of dual norm and $\int_{K \times K} \|X - Y\| d\nu \leq \delta$ for all Y whose distribution is in the Wasserstein ball $\mathcal{N}_\delta(\hat{\mu})$ we conclude that

$$R_\delta(A) \leq \frac{1}{N} \sum_{i=1}^N \|A - B_i\|_1 + \delta \|2A - 11^t\|_*$$

proving the inequality claimed in part (2) of the Theorem. Repeating the argument used in the proof of Theorem 1.3 we also conclude from equation (2) that

$$R_\delta(A) = \inf_{\lambda \geq 0} \left(\lambda \delta + \frac{1}{N} \sum_{i=1}^N \|A - B_i\|_1 + \frac{1}{N} \sum_{i=1}^N s_i \right)$$

where

$$\sup_{Y \in K} (\langle 2A - 11^t, B_i - Y \rangle - \lambda \|B_i - Y\|) \leq s_i$$

Using the definition of dual norm this inequality can be rewritten as

$$\sup_{Y \in K} \inf_{\|W\|_* \leq \lambda} \langle 2A - 11^t - W, B_i - Y \rangle \leq s_i$$

which by duality is equivalent to

$$\inf_{\|W\|_* \leq \lambda} \sup_{Y \in K} \langle 2A - 11^t - W, B_i - Y \rangle \leq s_i$$

which in turn is equivalent to the existence of a symmetric matrix W with $\|W\|_* \leq \lambda$ such that

$$\sup_{Y \in K} \langle 2A - 11^t - W, B_i - Y \rangle \leq s_i.$$

Moreover, letting $D = 2A - 11^t - W$ the previous inequality can be rewritten as

$$\sup_{Y \in K} \langle D, -Y \rangle \leq s_i - \langle D, B_i \rangle$$

and we will compute the supremum of the left-hand side using linear programming duality on the hypercube K . In $\mathcal{S}^{n \times n}$ the set K is defined by the restrictions $0 \leq Y \leq 11^t$ and thus the Lagrangian of our maximization problem is given by

$$L = \langle D, -Y \rangle + \langle \Lambda, 11^t - Y \rangle + \langle \eta, Y \rangle = \langle D + \Lambda - \eta, -Y \rangle + \langle \Lambda, 11^t \rangle$$

where the symmetric matrices $\Lambda, \eta \geq 0$. It follows that

$$\sup_{Y \in K} \langle -D, Y \rangle = \sup_{Y \in \mathcal{S}^{n \times n}} \inf_{\Lambda, \eta \geq 0} L$$

and exchanging infimum and supremum, we obtain

$$\sup_{Y \in K} \langle -D, Y \rangle = \inf_{\Lambda, \eta \geq 0} \sup_{Y \in K} L = \inf_{\Lambda, \eta \geq 0} \begin{cases} \langle \Lambda, 11^t \rangle & \text{if } D + \Lambda + \eta = 0 \\ \infty & \text{otherwise.} \end{cases}$$

which is equivalent to $\inf_{\Lambda \geq 0} \|\Lambda\|_1$ subject to $\Lambda, D + \Lambda \geq 0$, proving part (1) of the Theorem. If $\|\bullet\|$ is a semidefinitely representable function then so is the dual norm and therefore the feasible set of the optimization problem is the intersection of an SDr set and a polyhedron and thus an SDr set. Since the objective function is linear it is therefore a semidefinite programming problem as claimed. \square

Remark 2.4. We believe that the inequality in part (2) of the Theorem is in fact an equality under very mild assumptions. The idea that regularization algorithms naturally arise from Wasserstein robust formulations has appeared in the literature, see for instance [?].

Motivated by the inequality in part (2) of Theorem 1.4 we define the following semidefinite-programming algorithm for graph summarization given an independent sample B_1, \dots, B_N of \mathcal{G} ,

Definition 2.5. *Given $\delta > 0$, the Wasserstein robust nuclear norm graph summarization (WRNS) algorithm consists of finding a matrix $\bar{A} \in \arg \min_{A \in K} \Delta(A)$ where*

$$\Delta(A) := \delta \|2A - 11^t\|_* + \frac{1}{N} \sum_{i=1}^N \|A - B_i\|_1$$

and $\|Z\|_*$ denotes the nuclear norm of a matrix Z defined as the sum of its singular values (since Z is symmetric this quantity coincides with the sum of the absolute values of the eigenvalues of Z).

3. EXACT COMMUNITY DETECTION IN THE STOCHASTIC BLOCK MODEL AND THE WASSERSTEIN NUCLEAR NORM.

In this Section we will prove that there is a choice of $\delta = \delta(N)$ such that the WRNS algorithm recovers the exact cluster structure of a random graph \mathcal{G} generated with the stochastic block model with very high probability.

More precisely suppose C_1, \dots, C_ℓ are a partition of the set $[n]$ and the real numbers p_i, q satisfy the inequalities $0 \leq q < \frac{1}{2} < p_i \leq 1$ for $i = 1, \dots, \ell$. We say that a random graph \mathcal{G} with vertex set $[n]$ is generated by the stochastic block model determined by the clusters C_1, \dots, C_ℓ and the numbers p_i, \bar{p} if the edges of \mathcal{G} are independent random variables and an edge joins vertices i, j with probability p_t if $\{i, j\} \subseteq C_t$ for some cluster C_t and with probability q if $\{i, j\}$ is not contained in any C_t .

By Lemma 2.2 the graph \mathcal{G} has a unique cluster (or community) structure A^* with entries in $\{0, 1\}$ given by $A_{ij}^* = 1$ iff $\{i, j\} \subseteq C_t$ for some cluster t . Given a random sample B_1, \dots, B_N , a (deterministic) graph summarization algorithm produces a symmetric matrix $\bar{A}(B_1, \dots, B_N)$ which is a random variable due to the randomness of the sample. We would like to understand how often does the algorithm recover the exact cluster structure, equivalently we would like to understand the probability that $\bar{A} = A^*$.

Our analysis of the WRNS algorithm will consist of two steps. In Section 3.1 we will find geometric conditions on the subdifferential of $\Delta(A)$ at A^* which guarantee that A^* is the unique solution of the optimization problem. These conditions provide a geometric explanation of the usefulness of the regularizer. These geometric conditions will depend on the sample and in Section 3.2 we will show that the probability that these conditions fail to hold decreases exponentially on the sample size N when δ is appropriately chosen.

3.1. Geometry of subdifferentials and sufficient conditions for exactness.

In this section we will study some basic properties of the subdifferential of $\Delta(A)$. Recall that if h is a real valued convex function on a real inner product space V then the subdifferential of h at a point $a \in \text{dom}(h)$ is the closed convex set given by

$$\partial h(a) := \{g \in V : \forall z \in \text{dom}(h) (h(z) \geq h(a) + \langle g, z - a \rangle)\}.$$

Subdifferentials are a very useful tool for proving that a point x^* is a minimizer of h because this occurs if and only if $\vec{0} \in \partial h(x^*)$.

Recall that

$$\Delta(A) = \delta \|2A - 11^t\|_* + \frac{1}{N} \sum_{k=1}^N \|A - B_k\|_1$$

And define functions f, g by

$$f(A) := \frac{1}{N} \sum_{k=1}^N \|A - B_k\|_1, \quad g(A) := \delta \|2A - 11^t\|_*$$

For vertices $i, j \in [n]$ let $n_1(ij)$ (resp. $n_0(ij)$) be the random variable which counts the number of times that a given pair is (resp is not) an edge of some B_k with $k =$

$1, \dots, N$ and let Γ be the symmetric matrix with entries given by $\Gamma_{ij} = \frac{n_0(ij) - n_1(ij)}{N}$. Finally let $I := \{(i, j) : \exists t \in \{1, \dots, \ell\} (\{i, j\} \subseteq C_t)\}$ and let $O = [n] \times [n] \setminus I$ so I contains edges which belong to some cluster while O contains all edges which connect distinct clusters. Henceforth we will adopt the convention that adjacency matrices have diagonal entries equal to one and in particular $\Gamma_{ii} = -1$ for all i .

The following Lemma summarizes some basic subdifferential properties of the functions f and g at A^* . Define the matrix $H^* := 2A^* - 11^t$ so H^* is an $\ell \times \ell$ block-matrix whose blocks correspond to the clusters. The diagonal blocks of H^* have all entries equal to 1 and all the off-diagonal blocks have all entries equal to -1 .

Lemma 3.1. *The following statements hold:*

- (1) *The subdifferential of f at A^* is the set of symmetric matrices C satisfying the inequalities*

$$\begin{cases} -1 \leq C_{ij} \leq 1, & \text{if } i = j, \\ \Gamma_{ij} \leq C_{ij} \leq 1, & \text{if } \{i, j\} \in I, i \neq j \\ -1 \leq C_{ij} \leq \Gamma_{ij}, & \text{if } \{i, j\} \in O. \end{cases}$$

- (2) *The subdifferential of g at A^* is the set of symmetric matrices C which satisfy $\|C\| \leq 2\delta$ and the equality $\langle C, H^* \rangle = 2\delta \|H^*\|_*$.*

Proof. (1) Since the subdifferential is additive it suffices to understand the subdifferential of the absolute value which is given by

$$\partial(|x - a|)(b) = \begin{cases} 1, & \text{if } b > a \\ [-1, 1], & \text{if } b = a \\ -1, & \text{if } b < a \end{cases}$$

If $i, j \in C_t$ with $i \neq j$ then $A_{ij}^* = 1$ and the entry ij of the subdifferential of the sum at A^* is $[-1, 1]$ for each B_k containing the edge and it is 1 for each B_k for which ij is not an edge. If $i = j$ then the entry ii of the subdifferential at A^* is $[-1, 1]$ leading to the inequality $-1 \leq C_{ii} \leq 1$. Finally i, j is not contained in any cluster then $A_{ij}^* = 0$ and the entry ij of the subdifferential of the sum at A^* is -1 for each B_k which contains the edge ij and $[-1, 1]$ for each B_k which does not, proving the claim. (2) It follows from the definition of subdifferential that for any norm $\|\bullet\|$ and any point X the subdifferential of the norm at X is given by those C for which the dual norm $\|C\|_* \leq 1$ and $\langle C, X \rangle = \|X\|$ from which claim (2) follows immediately. \square

To simplify the inequalities in the previous Theorem we define a linear operator $\tilde{\bullet} : \mathcal{S}^{n \times n} \rightarrow \mathcal{S}^{n \times n}$ on symmetric matrices by the formula:

$$\tilde{A} = \begin{cases} A_{ij} & \text{if } i = j \text{ or } ij \in I \text{ and} \\ -A_{ij} & \text{if } ij \in O. \end{cases}$$

The operator $\tilde{\bullet}$ is an involution which satisfies $\langle A, B \rangle = \langle \tilde{A}, \tilde{B} \rangle$ for any two symmetric matrices A and B . Moreover using this operator, the previous Lemma can be restated by saying that C_{ij} belongs to the subdifferential of f at A^* if and only if $\tilde{\Gamma}_{ij} \leq \tilde{C}_{ij} \leq 1$ for all i, j . Note also that $\tilde{H}^* = 11^t$

Our next Lemma gives sufficient conditions for the true cluster structure A^* to be a minimizer of $\Delta(A)$ in K . In order to describe it we introduce the following two quantities.

Definition 3.2. *Let δ be a positive real number. For a symmetric matrix Γ define the quantities*

$$b(\Gamma, \delta) := \sum_{i \neq j} \max \left(\widetilde{\Gamma}_{ij} + \frac{2\delta}{n}, 0 \right) \text{ and } a(\Gamma, \delta) := \sum_{i \neq j} \max \left(-\widetilde{\Gamma}_{ij} - \frac{2\delta}{n}, 0 \right)$$

The quantity $b(\Gamma, \delta)$ (resp. $a(\Gamma, \delta)$) measures the total amount by which the matrix $-\frac{2\delta}{n}H^* = -\frac{2\delta}{n}11^t$ fails (resp. succeeds) to be in the subdifferential of Lemma 3.1. This is because $b(\Gamma, \delta)$ (resp. $a(\Gamma, \delta)$) is the result of summing over all ij the amount by which the inequalities $\widetilde{\Gamma}_{ij} \leq \frac{2\delta}{n}11^t$ fail (resp. succeed). The key point of the following Theorem is that if the inequality fails by less than it succeeds then the subdifferential of the spectral norm is sufficiently rich so as to allow us to redistribute these quantities using transportation matrices. In this sense the following Theorem explains the success of the spectral norm in cluster recovery algorithms.

For ease of exposition we will split the proof into two parts. First we will prove that this occurs when our graph involves only two clusters and then will generalize the result to any number $l \geq 2$ of clusters.

We will use that $\langle H^*, H^* \rangle = n^2$ and that the equalities $\|H^*\|_* = \|H\| = n$ hold when there are only two clusters.

Lemma 3.3. *Assume there are only two clusters. Let $\delta > 0$ with $(\frac{\delta}{n} + b(\Gamma, \delta)) < \frac{N}{2}$. If $b(\Gamma, \delta) < \min(\delta, a(\Gamma, \delta))$ then A^* is a minimizer of the optimization problem $\min_A \Delta(A)$.*

Proof. We will construct a matrix C such that $-C \in \partial(g)(A^*)$ and $C \in \partial(f)(A^*)$. As a result $0 = C - C$ belongs to the subdifferential $\partial(\Delta)(A^*)$ proving that A^* is a minimizer of $\Delta(A)$ as claimed. As a first candidate for C we could choose $C = -\frac{2\delta}{n}H^*$. Since

$$-\frac{2\delta}{n} \langle H^*, H^* \rangle = -\frac{2\delta}{n} n^2 = -2\delta n \text{ and } \|C\| = \frac{2\delta}{n} \|H^*\| = 2\delta.$$

we conclude that $-C \in \partial g(A^*)$. Moreover $C \in \partial f(A^*)$ precisely if $\widetilde{\Gamma}_{ij} \leq \widetilde{C}_{ij} = -\frac{2\delta}{n} \leq 1$ for all ij . In general, the first inequality need not hold and we can split the entries ij into two sets U and V where this inequality is valid or (strictly) fails respectively. More precisely, define

$$U = \left\{ (i, j) : i \neq j \text{ and } \widetilde{\Gamma}_{ij} \leq -\frac{2\delta}{n} \right\} \text{ and } V = \left\{ (i, j) : i \neq j \text{ and } \widetilde{\Gamma}_{ij} > -\frac{2\delta}{n} \right\}$$

and note that

$$a(\Gamma, \delta) = - \sum_{ij \in U} \left(\widetilde{\Gamma}_{ij} + \frac{2\delta}{n} \right) \text{ and } b(\Gamma, \delta) = \sum_{ij \in V} \widetilde{\Gamma}_{ij} + \frac{2\delta}{n}.$$

If $b(\Gamma, \delta) < a(\Gamma, \delta)$ then we could modify the matrix \widetilde{C} by increasing the entries of \widetilde{C} in V and decreasing those in U by the same amount by adding transportation

matrices so as to make the inequality valid in all entries. In the remainder of the proof we show that this process can be carried out while at the same time controlling the spectral norm of C .

Since $b(\Gamma, \delta) < a(\Gamma, \delta)$ there exist nonnegative scalars γ_{ij}^{st} for $ij \in U$ and $st \in V$ which tell us how much of the amount in entry $ij \in U$ has to be moved to entry $st \in V$. These numbers satisfy the following inequalities:

$$(3) \quad \forall st \in V \left(\widetilde{\Gamma}_{st} \leq -\frac{2\delta}{n} + \sum_{ij \in U} \gamma_{ij}^{st} \right) \text{ and } \forall st \in U \left(\widetilde{\Gamma}_{st} \leq -\frac{2\delta}{n} - \sum_{ij \in V} \gamma_{ij}^{st} \right).$$

In order to transport the smallest possible total amount we can moreover assume that the γ_{ij}^{st} are chosen so the first inequality is an equality.

$$\forall st \in V \left(\widetilde{\Gamma}_{st} = -\frac{2\delta}{n} + \sum_{ij \in U} \gamma_{ij}^{st} \right)$$

For $st \in V$ define $W^{st} = \sum_{ij \in U} \gamma_{ij}^{st} (r_{st} - r_{ij})$ where r_{st} is the $n \times n$ symmetric matrix given by

$$(r_{ij})_{ab} = \begin{cases} -1, & \text{if } (a, b) = (i, i) \text{ or } (a, b) = (j, j) \\ 1, & \text{if } (a, b) = (i, j) \text{ or } (a, b) = (j, i) \\ 0, & \text{else.} \end{cases}$$

and let $C := -\frac{2\delta}{n}H^* + \sum_{st \in V} \widetilde{W}^{st}$. We will show that $C \in \partial f(A^*)$ and that $-C \in \partial g(A^*)$ finishing the proof of the Theorem. Since $\widetilde{C} = -\frac{2\delta}{n}11^t + \sum_{st \in V} W^{st}$ we know that

$$\widetilde{C}_{ab} = \begin{cases} -\frac{2\delta}{n} + \sum_{ij \in U} \gamma_{ij}^{ab} & \text{if } ab \in V \\ -\frac{2\delta}{n} - \sum_{ij \in V} \gamma_{ij}^{ab} & \text{if } ab \in U \\ -\frac{2\delta}{n} - \sum_{st \in V} \sum_{aj \in U} \gamma_{aj}^{st} + \sum_{ij \in U} \sum_{at \in V} \gamma_{ij}^{at} & \text{if } a = b \end{cases}$$

we conclude that $\widetilde{\Gamma}_{ab} \leq \widetilde{C}_{ab} \leq 1$ for $a \neq b$. The first inequality follows from those in (3). The second inequality follows since for $ab \in V$ we have $\widetilde{C}_{ab} = \widetilde{\Gamma}_{ab} \leq 1$ and for $ab \in U$ we have $\widetilde{C}_{ab} \leq -\frac{2\delta}{n} \leq 1$.

♣♣♣ Mauricio: [PROBLEMA DIAGONAL: Queríamos demostrar que \widetilde{C} esta en el subdiferencial de f en A^* . Nos falta chequear la diagonal. Creo que lo que podemos demostrar es que se permiten ciertos tipos de transportes en los que no se mueve demasiada masa. Mejor aún, sera que siempre existe un transporte útil? Por útil quiero decir qu la suma con $a = b$ sea pequeña para todo vértice i . Esa suma se puede interpretar así: en un vértice a del grafo llamemos positivas a las aristas en V y negativas a las aristas en U (porque de U quitamos masa y en V la subimos. Lo que la suma mide es: cuánto sumamos en las aristas que tienen mas menos la cantidad que restamos (en valor absoluto) de las aristas que tienen menos. Eso podría pensarse como el "badness" de un vértice. La suma de los badness de todos los vértices es el doble del badness total (porque toda arista tiene dos vértices). Asi que concluimos que el transporte es válido

(la matriz C estará en el subdiferencial) si y solo si para todo vértice el badness del vértice respecto al transporte γ_{ij}^{st} cumple que $|b_v - \frac{2\delta}{n}| \leq 1$

]

Moreover, we know that

$$\langle C, H^* \rangle = \langle \widetilde{C}, \widetilde{H}^* \rangle = \left\langle -\frac{2\delta}{n} 11^t - \sum_{st \in V} W^{st}, 11^t \right\rangle = -2\delta n$$

where the last equality occurs since $\langle 11^t, r_{st} \rangle = 0$ for all st . For $i \neq j$ let $e^{ij} := \widetilde{r}_{ij}$ and note that the matrix e^{ij} satisfies the following properties:

- (1) $H^* e^{ij} = 0 = e^{ij} H^*$ for all ij . This is immediate from the fact that e^{ij} is given by

$$(e^{ij})_{ab} = \begin{cases} 1, & \text{if } ij \in I \text{ and } \{i, j\} = \{a, b\}. \\ -1, & \text{if } ij \in O \text{ and } \{i, j\} = \{a, b\} \\ -1, & \text{if } a = b \text{ and } a \in \{i, j\} \\ 0, & \text{otherwise.} \end{cases}$$

- (2) The inequality $\|e^{ij} - e^{st}\| \leq 2$ holds for all ij and st . This is immediate from the fact that the square of the spectral norm is bounded by the product of the induced 1-norm and the induced ∞ -norm. The inequality is strict only if $|\{i, j\} \cap \{s, t\}| \geq 1$ and in this case the norm of the difference takes the values of $\sqrt{3}$ and 0 when the intersection has sizes one and two respectively.

It follows from (1) that the two summands in $C = -\frac{2\delta}{n} H^* + \sum_{st \in V} \widetilde{W}^{st}$ are symmetric matrices with product zero. We conclude that they are simultaneously diagonalizable and that the spectral norm of C is given by

$$\|C\| = \max \left(\left\| \frac{2\delta}{n} H^* \right\|, \left\| \sum_{st \in V} \widetilde{W}^{st} \right\| \right)$$

by the triangle inequality and (2) the second term is bounded by $2b(\Gamma, \delta)$ and thus the spectral norm equals 2δ since $b(\Gamma, \delta) < \delta$. We conclude that $-C \in \partial g(A^*)$ as claimed. \square

Next we will now prove the case when there are any number of clusters. The proof will be similar that of the previous theorem. We will start with the candidate matrix $-\frac{2\delta}{n} H^*$ and correct it by adding transportation matrices that assure that the corrected matrix belongs to the subdifferential of $\Delta(A)$ at A^* . The difficulty in applying the tools of the previous theorem to solve the general case is that the matrices K that transport weight from one cluster to another do not, in general, satisfy the relation $KH^* = H^*K = 0$ when there are more than two clusters. This problem can be solved by splitting the matrix H^* into matrices than only take into account 2 clusters, and using the previous theorem. We begin recalling the following simple result:

Lemma 3.4. *Let $a_i, b_i \geq 0$, $i = 1, \dots, p$ be two non-negative, finite sequences of real numbers such that*

$$\sum_{i=1}^p a_i \geq \sum_{i=1}^p b_i.$$

Then there exist a finite sequence of reals c_i such that

- $\sum_{i=1}^p c_i = 0$.
- $a_i \geq b_i + c_i \forall i$.

Now we proceed to do the proof. For clusters $C_s \neq C_t$ define the matrix $H^{C_s C_t}$ whose entries are given by:

$$H_{uv}^{C_i C_j} = \begin{cases} 1 & \text{if } u, v \in C_s \text{ or } u, v \in C_t. \\ -1 & \text{if } u \in C_s, v \in C_t \text{ or } u \in C_s, v \in C_t. \\ 0 & \text{in any other case.} \end{cases}$$

Notice that this matrix has 4 blocks. Two with only 1 and two with only -1 . Moreover, its spectral norm is equal to $|C_s| + |C_t|$.

Theorem 3.5. *Suppose that $b(\Gamma, \delta) < \min(\delta, a(\Gamma, \delta))$. Then, A^* is a minimizer of the optimization problem $\min_A \Delta(A)$.*

Proof. Assume that there are l clusters. First of all, observe that

$$\frac{-2\delta}{n} H^* = \frac{-2\delta}{n} \frac{1}{l-1} \sum_{1 \leq s < t \leq l} H^{C_s C_t}.$$

For each, $C_s \neq C_t$ construct a transport matrix Δ_{st} as in the previous theorem, as to assure that $\Delta_{st} H^{C_s C_t} = H^{C_s C_t} \Delta_{st} = 0$. This can be done since $H^{C_s C_t}$ takes into account only two clusters. Recall that the total amount of weight to be corrected is $b(\Gamma, \delta)$. Let $w_{s,t}$ the weight to be distributed from cluster s to cluster t . In the notation of the previous theorem, w_{st} is just the sum of the $\gamma_{l_p}^{ij}$ where $l_p \in C_s$ and $ij \in C_t$.

Let

$$C := -\frac{2\delta}{n} H^* + \sum_{i < j} \Delta_{ij} = \frac{-2\delta}{n} \frac{1}{l-1} \sum_{1 \leq i < j \leq l} H^{C_i C_j} + \sum_{i < j} \Delta_{ij}$$

Finally, assume that for each $i < j$, $\frac{1}{l-1} \|H^{C_i C_j}\| \geq \|\Delta_{ij}\|$.

Then,

$$\begin{aligned} \|C\| &= \left\| \frac{-2\delta}{n} \frac{1}{l-1} \sum_{1 \leq i < j \leq l} H^{C_i C_j} + \sum_{i < j} \Delta_{ij} \right\| \\ &\leq \frac{2\delta}{n(l-1)} \sum_{1 \leq i < j \leq l} \left\| H^{C_i C_j} + \frac{n(l-1)}{2\delta} \Delta_{ij} \right\| \\ &= \frac{2\delta}{n(l-1)} \sum_{1 \leq i < j \leq l} \max(\|H^{C_i C_j}\|, \left\| \frac{n(l-1)}{2\delta} \Delta_{ij} \right\|) \end{aligned}$$

Now notice that

$$\begin{aligned} \delta \geq b(\Gamma, \delta) \text{ therefore } (l-1)n &\geq \frac{(l-1)n}{\delta} b(\Gamma, \delta) \\ \text{which implies that } \sum_{i < j} \|H^{C_i C_j}\| &\geq \frac{(l-1)n}{\delta} \sum_{i < j} w_{i,j} \\ &\geq \frac{(l-1)n}{2\delta} \sum_{i < j} \|\Delta_{i,j}\|. \end{aligned}$$

By the claim, we can assume without loss of generality that for each $i < j$,

$$\|H^{C_i, C_j}\| \geq \frac{(l-1)n}{\delta} \|\Delta_{i,j}\|.$$

This implies that the last sum reduces to

$$\frac{2\delta}{n(l-1)} \sum_{1 \leq i < j \leq l} \|H^{C_i C_j}\| = \sum_{1 \leq i < j \leq l} \frac{2\delta(|C_i| + |C_j|)}{n(l-1)} = \frac{2\delta(l-1)}{n(l-1)} \sum_{1 \leq i < j \leq l} |C_i| + |C_j| = 2\delta.$$

And so $\|C\| \leq 2\delta$.

□

♣♣♣ Daniel: [toca revisar que $\langle h^*, C \rangle$ es igual a $-2\delta n$ o eso es obvio?] ♣♣♣
Mauricio: [Toca revisar. Porfa revisa y me cuenta]

Uniqueness of the minimizer. In this brief section we discuss an important corollary: A^* is the unique minimizer of the optimization problem $\min_A \Delta(A)$. We begin by proving a well-known lemma for which we could not find a specific reference.

Lemma 3.6. *Let f be a convex function defined over a region D . Let \hat{x} be a point in its domain such that the subdifferential of f at \hat{x} is full dimensional and 0 belongs to its interior. Then, \hat{x} is the unique minimizer of f .*

Proof. Let $B_\epsilon(0)$ be a ball of radius ϵ centered in 0 and contained in $\partial(f)(\hat{x})$. Let $x \in D$ with $x \neq \hat{x}$. Let $Q \in \partial(f)(\hat{x})$. By the property of the elements of the subdifferential at a point,

$$f(x) \geq f(\hat{x}) + \langle Q, x - \hat{x} \rangle.$$

This property holds for every $Q \in \partial(f)(\hat{x})$, so taking supremum we obtain that

$$f(x) \geq \sup_{Q \in \partial(f)(\hat{x})} f(\hat{x}) + \langle Q, x - \hat{x} \rangle ..$$

Since $B_\epsilon(0) \subseteq \partial(f)(\hat{x})$ we obtain that

$$f(x) \geq f(\hat{x}) + \sup_{Q \in B_\epsilon(0)} \langle Q, x - \hat{x} \rangle = f(\hat{x}) + \epsilon \|x - \hat{x}\|.$$

As $x \neq \hat{x}$, $\epsilon \|x - \hat{x}\| > 0$. Therefore, $f(x) > f(\hat{x})$ for all $x \in D$ different of \hat{x} .

□

Remark 3.7. Under the conditions of theorem 3.3, The matrix C^1 we constructed satisfies the inequalities given by 3.1 strictly, so C^1 is an interior point of $\partial(f)(A^*)$. It follows that the matrix C constructed in 3.5 also satisfies these inequalities strictly and therefore it is also an interior point of $\partial(f)(A^*)$.

Corollary 3.8. *Under the conditions of Theorem 3.3, A^* is the unique minimizer of the optimization problem $\min_A \Delta(A)$.*

Proof. By 3.7, the matrix C constructed in 3.5 is an interior point of $\partial(f)(A^*)$. Therefore, as the subdifferential of Δ at A^* is equal to the Minkowski sum of the subdifferentials of g and f at A^* , $0 = C - C$ is an interior point of $\partial(\Delta)(A^*)$. It follows by lemma 3.6 that A^* is the unique minimizer of the optimization problem $\min_A \Delta(A)$. □

Using Theorem 3.3 we now estimate the probabilities of perfect recovery of the correct cluster structure.

3.2. A bound for recovery probabilities. In this section we will prove Theorem 1.5 which gives an upper bound on the probability that the correct A^* is not the unique optimal solution of our optimization problem. Our main tools will be concentration inequalities and in particular the ideas used in the proof of Hoeffding's inequality. Recall that Hoeffding's inequality says that if X_1, \dots, X_T are independent random variables with values in $[c_i, d_i]$ and $\Lambda_T := \sum_{i=1}^T X_i$ then the following holds for all $t \geq 0$

$$\mathbb{P}\{\Lambda_T - \mathbb{E}[\Lambda_T] \geq t\} \leq \exp\left(-\frac{2t^2}{\sum_{i=1}^T (d_i - c_i)^2}\right).$$

proof of Theorem 1.5. By Lemma 3.5 and the union bound the probability that A^* is not an optimal solution of problem (1.2) is bounded above by

$$(4) \quad \mathbb{P}\{b(\Gamma, \delta) \geq a(\Gamma, \delta)\} + \mathbb{P}\{b(\Gamma, \delta) \geq \delta\}.$$

and we will find upper bounds for the individual terms in (4). For $t = 1, \dots, N$ and $i, j \in [n]$ define

$$Z_{ij}^{(t)} := \begin{cases} -1, & \text{if } (B_t)_{ij} = 1 \\ +1, & \text{if } (B_t)_{ij} = 0 \end{cases}$$

and note that for every $i \neq j$ the equality $\sum_{t=1}^N \frac{Z_{ij}^{(t)}}{N} = \Gamma_{ij}$ holds. As a result

$$b(\Gamma, \delta) - a(\Gamma, \delta) = \sum_{i \neq j} \left(\widetilde{\Gamma}_{ij} + \frac{2\delta}{n} \right) = \frac{2\delta n(n-1)}{n} + \sum_{t=1}^N \sum_{i \neq j} \frac{\widetilde{Z_{ij}^{(t)}}}{N}$$

and therefore if $M := \mathbb{E} \left[\sum_{t=1}^N \sum_{i \neq j} \frac{\widetilde{Z_{ij}^{(t)}}}{N} \right]$ then the number M is negative and is given by the formula

$$M = (2q - 1)2|O| + \sum_{i=1}^l 2 \binom{c_i}{2} (1 - 2p_i) \leq -2\alpha n(n-1)$$

We can therefore bound the probability in the first term with

$$\begin{aligned} \mathbb{P} \left\{ \frac{2\delta n(n-1)}{n} + \sum_{t=1}^N \sum_{i \neq j} \frac{\widetilde{Z_{ij}^{(t)}}}{N} \geq 0 \right\} &= \mathbb{P} \left\{ \sum_{t=1}^N \sum_{i \neq j} \frac{\widetilde{Z_{ij}^{(t)}}}{N} - M \geq -2\delta(n-1) - M \right\} \leq \\ &\leq \exp \left(-2 \frac{(-M - 2\delta(n-1))^2}{Nn(n-1)(\frac{2}{N})^2} \right) = \exp \left(-\frac{N}{2} \left(1 - \frac{1}{n} \right) \left(\frac{-M}{n-1} - 2\delta \right)^2 \right) \end{aligned}$$

where the inequality follows from Hoeffding's inequality applied to the $Nn(n-1)$ independent random variables $\frac{\widetilde{Z_{ij}^{(t)}}}{N}$ which have values in $[-\frac{1}{N}, \frac{1}{N}]$. The inequality applies whenever $-\frac{M}{2(n-1)} > \delta > 0$. In particular whenever $0 < \delta < \alpha n$ we have

$$\mathbb{P}\{b(\Gamma, \delta) - a(\Gamma, \delta)\} \leq \exp \left(-\frac{2N(n-1)^3(\alpha n - \delta)^2}{n} \right).$$

Bounding the second term is more involved. Recall that

$$b(\Gamma, \delta) = \sum_{i \neq j} \max \left(\widetilde{\Gamma_{ij}} + \frac{2\delta}{n}, 0 \right).$$

Let $Y_{ij} := \widetilde{\Gamma_{ij}} + \frac{2\delta}{n}$ and let $X_{ij} := \max(Y_{ij}, 0)$. In order to prove a concentration inequality for the variables X_{ij} we begin by studying their moment generating functions $m_{X_{ij}}(t)$. Note that for every real number t the equality

$$\exp(tX_{ij}) = 1_{\{Y_{ij} \leq 0\}} + 1_{\{Y_{ij} \geq 0\}} \exp tY_{ij}$$

holds. Now $Y_{ij} = 1 + \frac{2\delta}{n} - 2\frac{n_{ij}}{N}$ where n_{ij} is a binomial random variable with parameters N and p_{ij} given by

$$p_{ij} := \begin{cases} p_t, & \text{if } \{i, j\} \subseteq C_t \\ 1 - q, & \text{else} \end{cases}$$

As a result taking expected values on both sides of the expression above we conclude that

$$m_{X_{ij}}(t) \leq \mathbb{P}\{Y_{ij} \leq 0\} + e^{t(1+\frac{2\delta}{n})} \mathbb{E} \left(e^{-\frac{2t}{N}n_{ij}} 1_{\{Y_{ij} \geq 0\}} \right).$$

Using the Cauchy-Schwartz inequality and the known formula for the moment generating function of a binomial random variable it follows that

$$\begin{aligned} m_{X_{ij}}(t) &\leq \mathbb{P}\{Y_{ij} \leq 0\} + e^{t(1+\frac{2\delta}{n})} \mathbb{E} \left(e^{-\frac{4t}{N}n_{ij}} \right)^{\frac{1}{2}} \mathbb{P}\{Y_{ij} \geq 0\}^{\frac{1}{2}} = \\ &= \mathbb{P}\{Y_{ij} \leq 0\} + e^{t(1+\frac{2\delta}{n})} \left(e^{-\frac{4t}{N}p_{ij}} + q_{ij} \right)^{\frac{N}{2}} \mathbb{P}\{Y_{ij} \geq 0\}^{\frac{1}{2}} \end{aligned}$$

where $q_{ij} := 1 - p_{ij}$. By Hoeffding's inequality on Bernoulli random variables we know that

$$\mathbb{P}\{Y_{ij} \geq 0\} \leq \exp\left(-\frac{N}{2}\left(-\frac{2\delta}{n} - (1 - 2p_{ij})\right)^2\right) \leq \exp(-2N(\alpha - \delta/n)^2)$$

so if $t = aN$ the inequality

$$e^{t(1+\frac{2\delta}{n})} \exp(-N(\alpha - \delta/n)^2) \leq 1$$

holds whenever $a \leq \frac{(\alpha - \delta/n)^2}{(1+\frac{2\delta}{n})}$ and for all such a we have

$$m_{X_{ij}}(aN) \leq \left(1 + (e^{-4a}p_{ij} + q_{ij})^{\frac{N}{2}}\right)$$

We define $a(\delta) := \frac{(\alpha - \delta/n)^2}{(1+\frac{2\delta}{n})}$ and will use it to prove a moment concentration inequality for $b(\Gamma, \delta)$ which will give us a bound on the second term in (4). For every $t > 0$ we have

$$\mathbb{P}\{b(\Gamma, \delta) \geq \delta\} = \mathbb{P}\left\{\exp\left(t \sum_{i \neq j} X_{ij}\right) \geq e^{t\delta}\right\} \leq e^{-t\delta} \prod_{i \neq j} \mathbb{E}[e^{tX_{ij}}] = e^{-t\delta} m_{X_{ij}}(t)$$

Choosing $t = a(\delta)N$ and using the previous inequality we see that

$$\mathbb{P}\{b(\Gamma, \delta) \geq \delta\} \leq e^{-N\delta a(\delta)} \prod_{i \neq j} \left(1 + (e^{-4a}p_{ij} + q_{ij})^{\frac{N}{2}}\right)$$

Which decreases exponentially in N for any $0 \leq \delta \leq n\alpha$. The rate of decrease of the first term is controlled by the positive factor

$$\delta a(\delta) = \frac{\delta \left(\alpha - \frac{\delta}{n}\right)^2}{\left(1 + \frac{2\delta}{n}\right)}.$$

and we let δ^* be a maximizer of this function. \square

4. AN ALGORITHM FOR WASSERSTEIN NUCLEAR NORM SUMMARIZATION

Solving the optimization problems appearing in Theorem 1.4 require solving large semidefinite programs which are beyond the capacity of standard off-the-shelf software even for relatively small graphs (of say 70 vertices with $N = 4$). One possible reason is that off-the-shelf solvers often use interior point methods, which are highly accurate but often do not scale well. A better alternative, especially well suited for solving is to use first order numerical optimization methods such as ADMM.

In this section, we provide an algorithm specially adapted for the Wasserstein nuclear norm summarization. It is based on a variation of the **Alternating Direction Method of Multipliers** (ADMM) called **Global Variable consensus with regularization**. Our algorithm is derived using the theory given in [6].

4.1. Global Variable consensus with regularization. The general form of Global Variable consensus with regularization is given by

$$(5) \quad \begin{aligned} & \text{Minimize } \sum_{i=1}^n f_i(x_i) + g(z) \\ & \text{Subject to: } x_i - z = 0, \quad i = 1, \dots, N. \end{aligned}$$

To efficiently solve this optimization problem, ADMM does iterative rounds of minimization of the primal and dual variables. For certain functions, (as is the case for the l_1 norm and crucially the nuclear norm) these minimizations problems have actual analytical minimizers.

The general algorithm to solve this optimization problem is given in [6] and consists of the following steps:

- (1) initialize x_i^0, y_i^0 for $i = 1, \dots, N$, $\rho > 0$ and z^0 .
- (2) Set $\bar{x}^k = \frac{1}{N} \sum_{i=1}^N x_i$ and $\bar{y}^k = \frac{1}{N} \sum_{i=1}^N y_i$.
- (3) $x_i^{k+1} = \arg \min_{x_i} (f_i(x_i) + \langle y_i^k, x_i - z^k \rangle) + \frac{\rho}{2} \|x_i - z^k\|_2^2$.
- (4) $z^{k+1} = \arg \min_z (g(z) + \frac{N\rho}{2} \|z^k - \bar{x}^{k+1} - \frac{1}{\rho} \bar{y}^k\|_2^2)$.
- (5) $y_i^{k+1} = y_i^k + \rho(x_i^{k+1} - z^{k+1})$.

This algorithm converges under very general circumstances, which can be easily checked for problem 1 :

Stopping criteria are derived using the dual and primal residuals [6]. For The Global Variable consensus with regularization, the primal residual on the k -step is:

$$r^k := (x_1^k - z^k, x_2^k - z^k, \dots, x_N^k - z^k)$$

and the dual residual in the k -step

$$s^k := -\rho(z^k - z^{k-1})$$

Given $\varepsilon_1, \varepsilon_2$, the stopping criteria is given by

$$\|r^k\|_2 \leq \varepsilon_1 \text{ and } s^k \leq \varepsilon_2.$$

4.2. Adapation to the Wasserstein nuclear norm summarization.

Definition 4.1. Let f be a convex function, $\rho > 0$. The proximal operator of f at w is defined as:

$$\text{prox}_{f,\rho}(w) = \arg \min_z f(z) + \frac{\rho}{2} \|z - w\|_2^2$$

Claim 4.2. if $\|\cdot\|_*$ denotes the nuclear norm, and if w is a matrix with singular value decomposition USV^t then,

$$UP_\epsilon V^t = \arg \min_x \epsilon \|x\|_* + \frac{1}{2} \|x - w\|_2^2.$$

Where

$$P_\epsilon = \begin{cases} x - \epsilon & \text{if } x > \epsilon \\ x + \epsilon & \text{if } x < -\epsilon \\ 0 & \text{in any other case.} \end{cases}$$

and P_ϵ is applied component-wise. P_ϵ is usually called the soft-thresholding operator.

Claim 4.3. if $\|\cdot\|_1$ denotes the l_1 norm, then

$$\text{prox}_{\|\cdot\|_1, \rho}(w) = \arg \min_x \|x\|_1 + \frac{\rho}{2} \|x - w\|_2^2 = P_{\frac{1}{\rho}}(w).$$

Where $P_{\frac{1}{\rho}}$ is applied component-wise. Moreover, if c is any $n \times n$ matrix, then

$$P_{\frac{1}{\rho}}(w) + c = \arg \min_x \|x - c\|_1 + \frac{\rho}{2} \|x - w\|_2^2.$$

Let B_1, \dots, B_N of an *i.i.d* sample of the random graph \mathcal{G} . Let n be the number of vertices of \mathcal{G} and $\mathbf{1}$ denote the vector $[1, \dots, 1]$ of length n . To use the formulation given in 5 to solve the problem we need the following change of variables:

- $C_i = 2B_i - \mathbf{1}\mathbf{1}^t$.
- $Z = 2A - \mathbf{1}\mathbf{1}^t$.
- $f_i(x_i) = \frac{1}{2} \|x_i - C_i\|_1$.
- $g(z) = \|z\|_*$.

Our optimization problem reduces to the one given in 5 and an algorithm to solve it is given by:

- (1) initialize $\rho > 0$, $x_i^0 = 0$, $y_i^0 = 0$, for $i = 1, \dots, N$ and $z_0 = \frac{1}{N} \sum_{i=1}^N C_i$.
- (2) Set $\bar{x}^k = \frac{1}{N} \sum_{i=1}^N x_i$ and $\bar{y}^k = \frac{1}{N} \sum_{i=1}^N y_i$.
- (3) $x_i^{k+1} = P_{\frac{1}{2\rho}}(z^k - \frac{1}{\rho} y_i^k - C_i) + C_i$
- (4) $z^{k+1} = UP_{\frac{\lambda}{N\rho}}(S)V^t$ with $USV^t = \text{SVD}(\bar{x}^{k+1} + \frac{1}{\rho} \bar{y}^k)$.
- (5) $y_i^{k+1} = y_i^k + \rho(x_i^{k+1} - z^{k+1})$.
- (6) Until stopping criteria is met.

4.3. Numerical simulations. Using the algorithm given in the previous section, we tested the recovery of graphs generated by the stochastic block model. To this end, we implemented an algorithm on Julia that creates random graph that are distributed according to the stochastic block model. The input parameters are the following:

- (1) n : the number of vertices of the graph.
- (2) k : the number of clusters of the graph.
- (3) q : the probability of connecting two vertices that do not belong to the same cluster.
- (4) p_i for $i = 1, \dots, k$: the probability of connecting two vertices that belong to the cluster i .

The output of this algorithm is the adjacency matrix of the generated graph.

We begin by testing our algorithm by generating 3 observations of a random graph which is distributed according to the stochastic block model and running our algorithm for different values of δ . Success of recovery will be evaluated by using the *error of recovery* which is given by the formula

$$\|A^* - \bar{A}\|_1$$

where A^* is the adjacency matrix of the underlying cluster structure and \bar{A} is the adjacency matrix of the recovered graph. We present one such plot in 1. Notice that the true graph structure is recovered for certain values of δ . This is intuitively clear from the Wasserstein robust formulation. If the size of the ball is too small, we won't capture the true distribution of the random graph. If it is too big, we will capture too many distributions and the worst case error will be high. Choosing a correct δ is of the utmost importance.

Remark 4.4. In practice, δ could be chosen by using a trial and error methodology, along with a cluster quality metric. One such metric is called the *silhouette*.

Fortunately, our simulations suggest that the region where one can choose δ to obtain perfect recovery grows as more observations are added: see figures on 4.

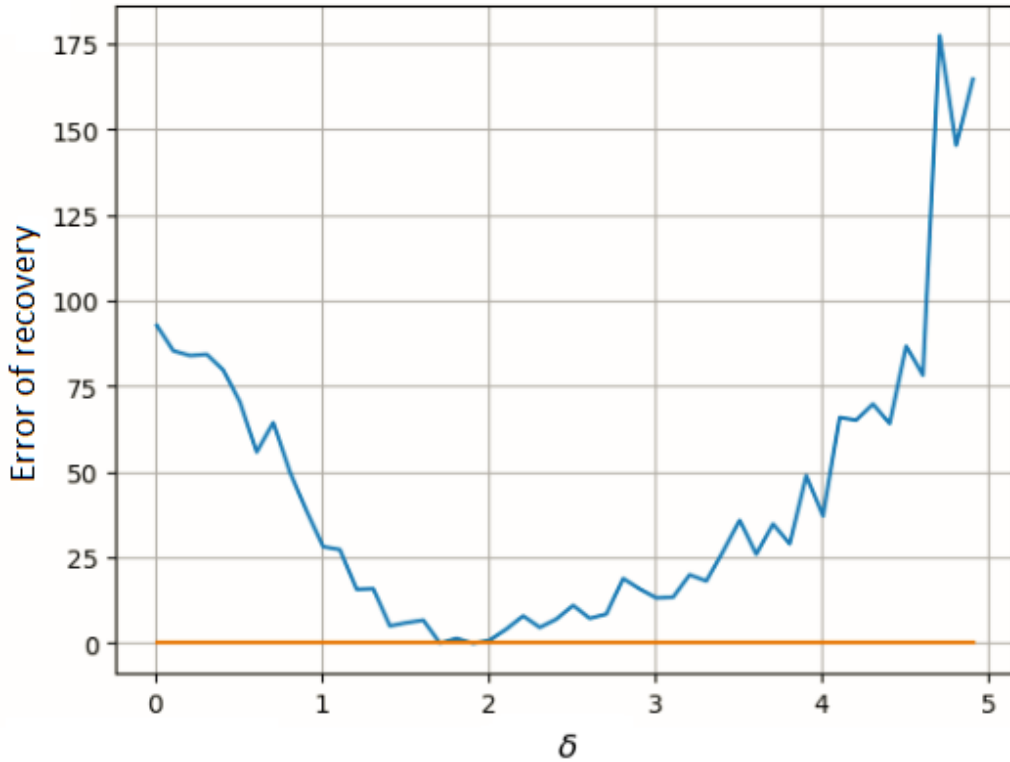


FIGURE 1. Recovery of the true cluster structure using 3 observations on a graph with generated with the stochastic block model with 2 clusters and 50 vertices.

As δ varies, the recovered graph changes as well. Figure 2 Shows the recovered graph for different values of δ . Note that a graph recovered by our algorithm has not necessarily entries in $\{0, 1\}$ and one might be tempted to round down the entries below certain threshold (say 0.4) and round up those above another threshold (say 0.6). However, it is not clear what we should do with entries between both thresholds.

Theorem 3.3 assures that as long as $p_i > 0.5$ and $q < 0.5$ the probability of perfect recovery converges to 1. The following experiments corroborate this result: We fix $n = 50$, $k = 2$, and let the first cluster have 15 vertices and the second one 35. We let $p = p_1 = p_2$ vary between 0.5 and 1 and q vary between 0 and 0.5. For each pair (p, q) , we generate N observations, run our algorithm and measure the error of recovery. We repeat this process 10 times and store the mean error of recovery in a matrix. We present the heat maps of such matrices in 3 for different values of N .

In theorem 3.3, the use of the spectral norm was crucial. Still, one might ask if other norms (say the 1-norm, 2-norm and ∞ -norm) can recover the underlying cluster structure.

To check this, We fix $n = 50$, $k = 2$ where the first cluster has 15 vertices and the second one has 35. We let $p_1 = p_2 = 0.70$ and $q = 0.2$. We compute the error of recovery for different values of δ . For recovery using the nuclear norm, we use the algorithm given in the previous section. For the 1-norm, 2-norm and ∞ -norm we use the *Mosek* implementation on Julia. We also include the error of recovery of the graph obtained by averaging the observations, which we call the mean graph. We repeat this experiment twice. First with 3 observations and then with 7. Results are shown in figure 4.

Notice that the error of recovery of the mean graph decreases as more observations are considered. It is still far off the true cluster structure even for 7 observations, even though with 3 observations we were already able to recover the true cluster structure using the nuclear norm.

An interesting question that needs to be addressed is that of the speed of convergence to the true cluster structure as N grows. If our algorithm needed to many observations of the random graph to find the cluster structure, we would simply use the mean of the observations. The following figures shows that this is not the case (at least for the stochastic block model), and thus there is a real benefit by using the Wasserstein summarization algorithm.

5. CONCLUSIONS AND FUTURE WORK

In this paper, we presented the general problem of finding deterministic summaries from an independent sample of a random graph \mathcal{G} . We then specialized this problem to the case of community detection and showed how the Wasserstein metric allows us to reformulate this problem as a robust optimization problem. We showed that if the Wasserstein distance is induced by the nuclear norm, we can recover the exact cluster structure of random graphs generated with the stochastic block model with overwhelming probability with very few samples. We presented a specific algorithm to solve the *Wasserstein robust nuclear norm summarization problem* and gave substantial simulations that corroborate our theoretical results.

Most importantly, we showed that a well studied problem in machine learning can be recast as a robust optimization problem using the Wasserstein metric. This approach is very promising, as it gives a principled approach to machine learning which oftentimes lacks a theoretical background (such as the trendy deep learning). For example, see [?]. This work is a small contribution to the growing body of applications of optimal transport to machine learning.

We conclude by briefly mentioning three interesting problems that rose in development of this work. **Sparse regime in community detection.** In the literature, the problem of finding communities in the stochastic block model when the graph is sparse is well studied. For example, see [20]. How does sparsity affect our results? We suspect that our algorithm are not well suited for sparse matrix since our methods are based on splitting the observations in sparse plus low rank matrices, and thus identifiability problems would rise if the observed matrices were sparse to begin with.

Arbitrary distribution of the Γ_{ij} . The quantities Γ_{ij} presented in 3.1 are random variables whose distribution is given by the properties of the stochastic block model. It would be interesting to study random graphs where the Γ_{ij} have an arbitrary distribution. This could lead to an application of our methods to weighted graphs, or to an appealing class of random graphs.

Graph summarization in an adversarial setting. It would be interesting to explore graph summarization on a broader setting. For example, we could consider an adversarial setting, where an adversary is presented a graph with a certain structure (for example a tree structure) and he generates a sample of graphs by removing or adding edges on the graph with probability $q < 1/2$. Can we recover the original graph given a very small sample? If so, which representable convex function would allow us to properly recover the structure (as is the case of the nuclear norm and the community structure)? Is it enough that such a function has a rich subdifferential as the nuclear norm so that some version of theorem 3.3 applies?

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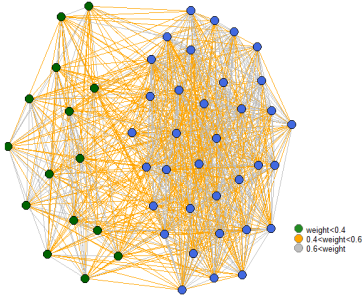
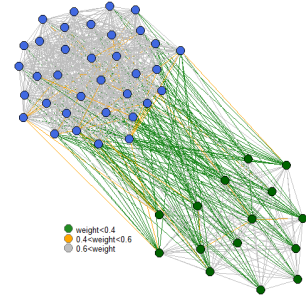
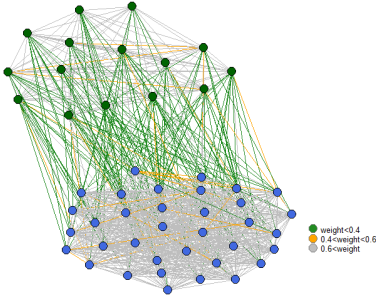
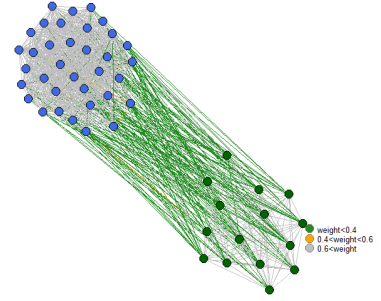
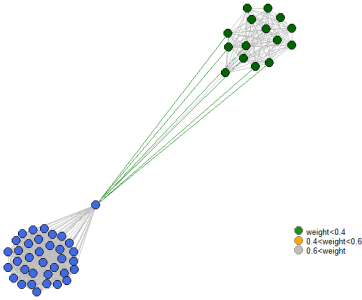
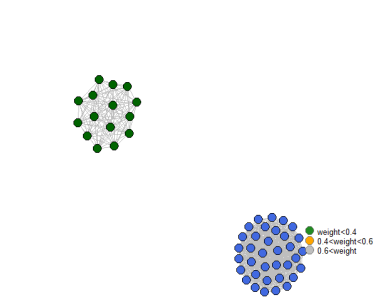
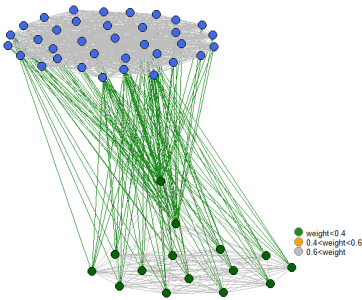
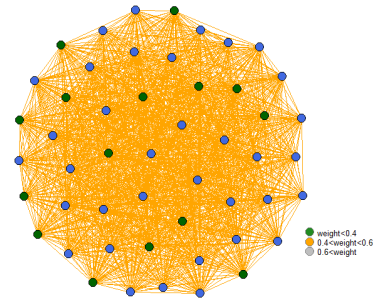
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(A) Recovery with $\delta = 0$ (B) Recovery with $\delta = 0.1$ (C) Recovery with $\delta = 0.5$ (D) Recovery with $\delta = 1.2$ (E) Recovery with $\delta = 1.5$ (F) Recovery with $\delta = 2$ (G) Recovery with $\delta = 11$ (H) Recovery with $\delta = 14$ FIGURE 2. Recovered graph from the same observations for different values of δ

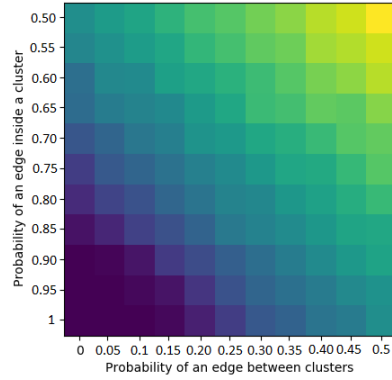
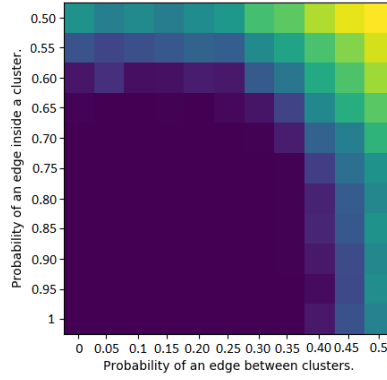
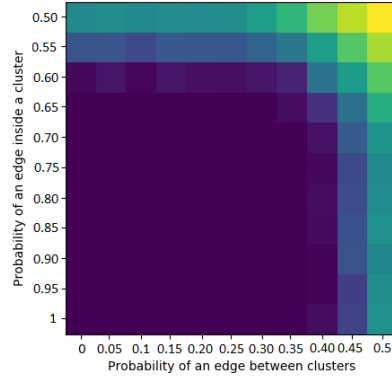
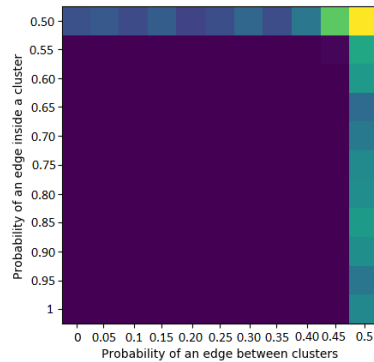
(A) $N = 1$ (B) $N = 3$ (C) $N = 7$ (D) $N = 25$

FIGURE 3. Simulation results for the average error of recovery (over 10 trials) for different values of p and q with N observations. $\delta = 1.5$ for the first two figures and 0.8 for the other two. Dark purple indicates

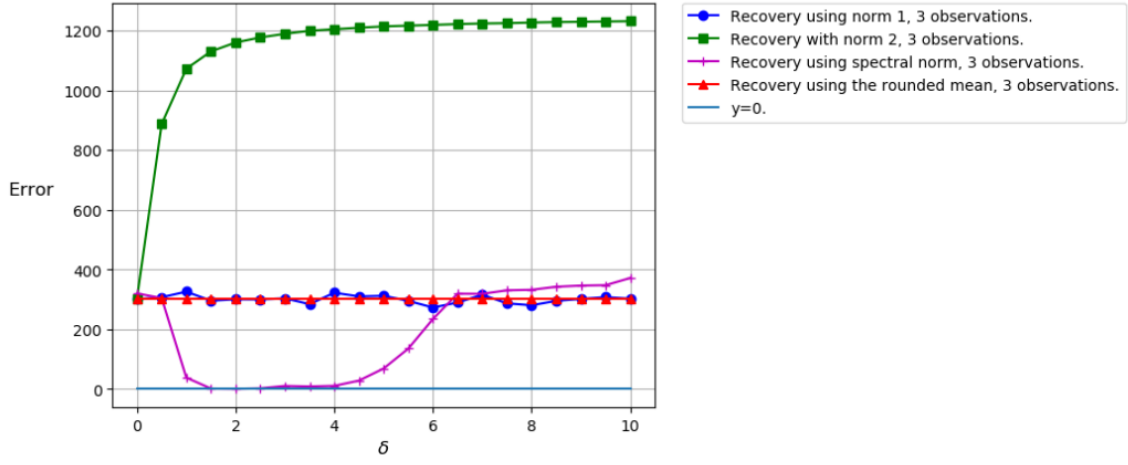
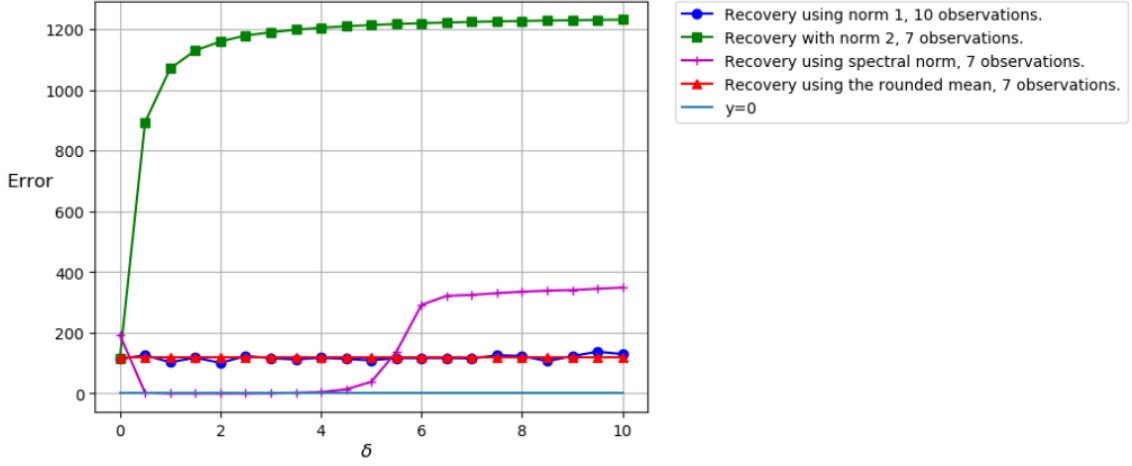
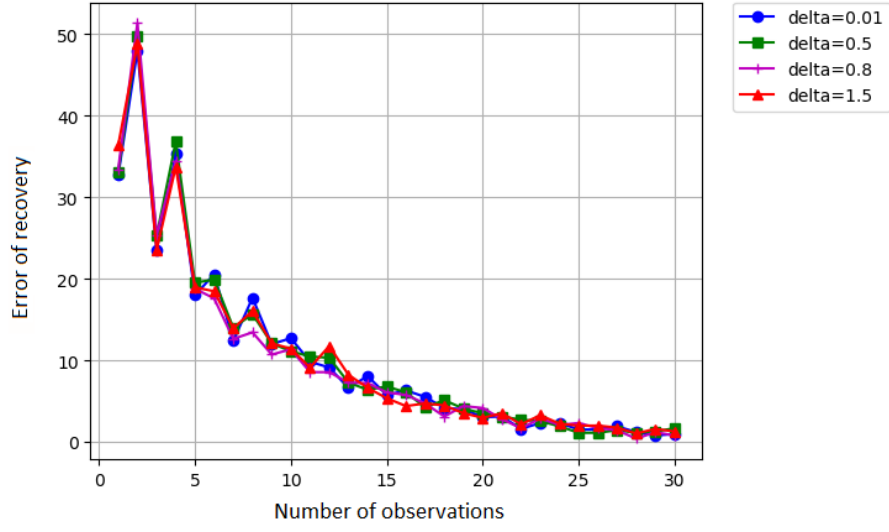
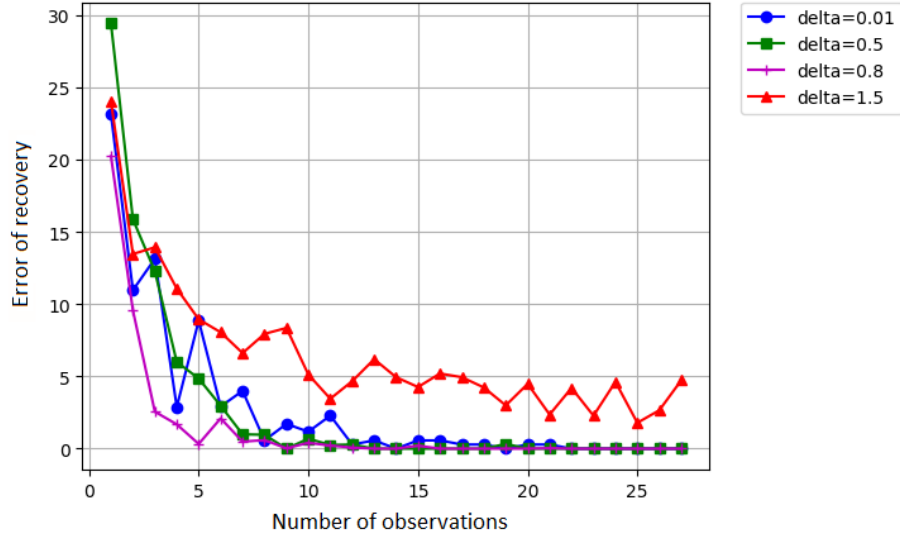
(A) $N = 3$ (B) $N = 7$

FIGURE 4. Error of recovery for different values of δ using the Wasserstein robust nuclear norm graph summarization and the l_1, l_2 norms as regularizers. The recovery error of the mean graph is also included.



(A) Error of recovery using the mean graph.



(B) Error of recovery using the Wasserstein robust nuclear norm graph summarization.

FIGURE 5. Simulation results for the speed of convergence to the true cluster structure of the Wasserstein robust nuclear norm graph summarization versus the mean graph summarization .