

Clustering and Parameter Estimation for the Popularity Adjusted Block Model

Abstract

In this paper, we connect two probabilistic models for graphs, the Popularity Adjusted Block Model (PABM) and the Generalized Random Dot Product Graph (GRDPG) and use properties established in this connection to aid in clustering and parameter estimation. In particular, we note that the PABM can be represented as latent positions such that points within the same cluster lie on a subspace, and the subspaces that represent each cluster are orthogonal to one another. Using this property as well as the asymptotic properties of Adjacency Spectral Embedding (ASE) of the GRDPG, we are able to establish theoretical asymptotic results of our clustering and parameter estimation methods for the PABM.

1 Introduction

One popular probabilistic model for graphs with underlying communities is the Stochastic Block Model (SBM), which assumes that the edge probability from one cluster to another follows a Bernoulli distribution with a fixed probability for each pair of communities. The Popularity Adjusted Block Model (PABM) was introduced by Sengupta and Chen [4] as a generalization of the SBM to address the heterogeneity of edge probabilities within and between communities or clusters while still maintaining the community structure.

The Random Dot Product Graph (RDPG) [1] is another probabilistic model with Bernoulli edge probabilities. Under this model, each vertex of the graph can be represented by a point in latent space such that the edge probability between any pair of vertices is given by their corresponding dot product in the latent space. The SBM is equivalent to a special case of the RDPG model in which all vertices in a given community share the same position in the latent space. It has also been shown that similar probabilistic graph models, (such as the Mixed Membership Stochastic Block Model [3]). An analogous property exists for the PABM not under the RDPG model but under the *Generalized* Random Dot Product Graph model.

1.1 Previous work

Noroozi, Rimal, and Pensky [2] proposed using sparse subspace clustering (SSC) to identify the cluster memberships given either an edge probability matrix P or an adjacency matrix A . In the case that P is known, the cluster memberships can be identified exactly (up to permutation). A similar procedure can be applied if P is unknown and we have an observation A , but the theoretical guarantees of this method applied to the PABM are unknown. In particular, the method requires spherical Gaussian noise. The authors of this paper then use point estimators for $\{\lambda^{(kl)}\}$ using cluster labels obtained via SSC.

2 Connecting the Popularity Adjusted Block Model to the Generalized Random Dot Product Graph

2.1 The popularity adjusted block model (PABM) [2]

Definition 1. Let $G = (V, E)$ be an undirected, unweighted random graph with corresponding affinity matrix $A \in \{0, 1\}^{n \times n}$. Then A is a random matrix with corresponding edge probability matrix P such that $A_{ij} \stackrel{\text{indep}}{\sim} \text{Bernoulli}(P_{ij})$ for $i > j$ ($A_{ji} = A_{ij}$ and $A_{ii} = 0$). Let there exist K underlying communities in G , and let n_k be the size of the k^{th} community in G such that $\sum_{k=1}^K n_k = n$.

If A and P are organized such that $n_k \times n_l$ blocks $A^{(kl)}$ and $P^{(kl)}$ describe the edges and edge probabilities between communities k and l , then $P^{(kl)} = \lambda^{(kl)}(\lambda^{(lk)})^\top$ for a set of fixed vectors $\{\lambda^{(st)}\}_{s,t=1,\dots,K}$. Each $\lambda^{(st)}$ for $s, t = 1, \dots, K$ is a column vector of length n_s (i.e., the community corresponding to the first index provides the vector length).

We will use the notation $A \sim PABM(\{\lambda^{(kl)}\}_K)$ to denote a random affinity matrix A drawn from a PABM with parameters $\lambda^{(kl)}$ consisting of K underlying clusters/communities.

2.2 The generalized random dot product graph (GRDPG) [3]

Definition 2. Let $X \in \mathbb{R}^{n \times d}$ be latent positions of the vertices of a graph G . X consists of row vectors x_i^\top . Let $A \in \{0, 1\}^{n \times n}$ be the corresponding affinity matrix.

Fix p, q such that $p + q = d$ and define $I_{pq} = \begin{bmatrix} I_p & 0 \\ 0 & -I_q \end{bmatrix}$.

Then $G = (V, E)$ is a generalized random dot product graph with signature (p, q) and latent positions X iff its random affinity matrix can be described as $A_{ij} \stackrel{\text{indep}}{\sim} \text{Bernoulli}(P_{ij})$ where $P_{ij} = x_i^\top I_{pq} x_j$.

We will use the notation $A \sim GRDPG_{p,q}(X)$ to denote a random affinity matrix A drawn from latent positions X and signature (p, q) .

Remark. Like the RDPG, the latent positions of a GRDPG are not unique. More specifically, if $P_{ij} = x_i^\top I_{pq} x_j$, then we also have for any $Q \in \{R : R^\top I_{pq} R = I_{pq}\}$, $(Qx_i)^\top I_{pq} (Qx_j) = x_i^\top (Q^\top I_{pq} Q) x_j = x_i^\top I_{pq} x_j = P_{ij}$ (this is the indefinite orthogonal group, $\mathbb{O}(p, q)$). Unlike in the RDPG case, transforming the latent positions by multiplication with $Q \in \mathbb{O}(p, q)$ does not necessarily maintain interpoint angles or distances.

2.3 Connecting the PABM to the GRDPG

2.3.1 Case where $K = 2$

Theorem 1. Let $X = \begin{bmatrix} \lambda^{(11)} & \lambda^{(12)} & 0 & 0 \\ 0 & 0 & \lambda^{(21)} & \lambda^{(22)} \end{bmatrix}$, and let $U = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1/\sqrt{2} & 1/\sqrt{2} \\ 0 & 0 & 1/\sqrt{2} & -1/\sqrt{2} \\ 0 & 1 & 0 & 0 \end{bmatrix}$, as in Definition

1. Then $A \sim GRDPG_{3,1}(XU)$ and $A \sim PABM(\{\lambda^{(kl)}\}_K)$ are equivalent.

Proof. Let $X = \begin{bmatrix} \lambda^{(11)} & \lambda^{(12)} & 0 & 0 \\ 0 & 0 & \lambda^{(21)} & \lambda^{(22)} \end{bmatrix}$ and $Y = \begin{bmatrix} \lambda^{(11)} & 0 & \lambda^{(12)} & 0 \\ 0 & \lambda^{(21)} & 0 & \lambda^{(22)} \end{bmatrix}$. Then $P = XY^\top$.

We can note that $Y = X\Pi$ where Π is the permutation matrix $\Pi = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$. Therefore, $P = X\Pi X^\top$.

Taking the spectral decomposition of $\Pi = UDU^\top$, we can see that $P = (XU)D(XU)^\top$. We can then denote $\Sigma = |D|^{1/2}$, the square root of the absolute values of the (diagonal) entries of D and obtain $P = (XU\Sigma)I_{pq}(XU\Sigma)^\top$ where p and q correspond to the number of positive and negative eigenvalues of Π , respectively. Therefore, the PABM with $K = 2$ is a special case of the GRDPG. We can however expand upon this a bit further.

The permutation described by Π has two fixed points and one cycle of order 2. The two fixed points are at positions 1 and 4, so Π has two eigenvalues equal to 1 and corresponding eigenvectors e_1 and e_4 . The cycle of order 2 switching positions 2 and 3 corresponds to eigenvalues 1 and -1 with corresponding

eigenvalues $(e_2 + e_3)/\sqrt{2}$ and $(e_2 - e_3)/\sqrt{2}$ respectively. Therefore, $D = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix} = I_{3,1}$ and

$$U = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1/\sqrt{2} & 1/\sqrt{2} \\ 0 & 0 & 1/\sqrt{2} & -1/\sqrt{2} \\ 0 & 1 & 0 & 0 \end{bmatrix}.$$

Putting it all together, we get $P = (XU)I_{3,1}(XU)^\top$. Therefore, the PABM with $K = 2$ is a GRDPG with $p = 3, q = 1, d = K^2 = 4$, and latent positions $XU = \begin{bmatrix} \lambda^{(11)} & 0 & \lambda^{(12)}/\sqrt{2} & \lambda^{(12)}/\sqrt{2} \\ 0 & \lambda^{(22)} & \lambda^{(21)}/\sqrt{2} & -\lambda^{(21)}/\sqrt{2} \end{bmatrix}$.

2.3.2 Generalization to $K > 2$

Theorem 2. There exists a block diagonal matrix $X \in \mathbb{R}^{n \times K^2}$ defined by PABM parameters $\{\lambda^{(kl)}\}_K$ and $U \in \mathbb{R}^{K^2 \times K^2}$ that is fixed for each K such that $A \sim \text{GRDPG}_{K(K+1)/2, K(K-1)/2}(XU)$ and $A \sim \text{PABM}(\{(\lambda^{(kl)})\}_K)$ are equivalent.

Proof Let $\Lambda^{(k)} = [\lambda^{(k,1)} \ \dots \ \lambda^{(k,K)}] \in \mathbb{R}^{n_k \times K}$.

Let X be a block diagonal matrix $X = \text{diag}(\Lambda^{(1)}, \dots, \Lambda^{(K)}) \in \mathbb{R}^{n \times K^2}$.

Let $L^{(k)}$ be a block diagonal matrix of column vectors $\lambda^{(lk)}$ for $l = 1, \dots, K$. $L^{(k)} = \text{diag}(\lambda^{(1k)}, \dots, \lambda^{(Kk)}) \in \mathbb{R}^{n \times K}$.

Let $Y = [L^{(1)} \ \dots \ L^{(K)}] \in \mathbb{R}^{n \times K^2}$.

Then $P = XY^\top$.

Similar to the $K = 2$ case, we again have $Y = X\Pi$ for a permutation matrix Π , so $P = X\Pi X^\top$.

The permutation described by Π has K fixed points, which correspond to K eigenvalues equal to 1 with corresponding eigenvectors e_k where $k = r(K+1) + 1$ for $r = 0, \dots, K-1$. It also has $\binom{K}{2} = K(K-1)/2$ cycles of order 2. Each cycle corresponds to a pair of eigenvalues $+1$ and -1 and a pair of eigenvectors $(e_s + e_t)/\sqrt{2}$ and $(e_s - e_t)/\sqrt{2}$.

So Π has $K(K+1)/2$ eigenvalues equal to 1 and $K(K-1)/2$ eigenvalues equal to -1 . Π has the decomposed form $\Pi = UI_{K(K+1)/2, K(K-1)/2}U^\top$, and we can describe the PABM with K communities as a GRDPG with latent positions XU with signature $(K(K+1)/2, K(K-1)/2)$.

Example for $K = 3$. Using the same notation as before:

$$X = \begin{bmatrix} \lambda^{(11)} & \lambda^{(12)} & \lambda^{(13)} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \lambda^{(21)} & \lambda^{(22)} & \lambda^{(23)} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \lambda^{(31)} & \lambda^{(32)} & \lambda^{(33)} \end{bmatrix}$$

$$Y = \begin{bmatrix} \lambda^{(11)} & 0 & 0 & \lambda^{(12)} & 0 & 0 & \lambda^{(13)} & 0 & 0 \\ 0 & \lambda^{(21)} & 0 & 0 & \lambda^{(22)} & 0 & 0 & \lambda^{(23)} & 0 \\ 0 & 0 & \lambda^{(31)} & 0 & 0 & \lambda^{(32)} & 0 & 0 & \lambda^{(33)} \end{bmatrix}$$

$$\text{Then } P = XY^\top \text{ and } Y = X\Pi \text{ where } \Pi = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

Another way to look at this is:

- Positions 1, 5, 9 are fixed
- The cycles of order 2 are
 - (2, 4)
 - (3, 7)
 - (6, 8)

Therefore, we can decompose $\Pi = UI_{6,3}U^\top$ where the first three columns of U consist of e_1 , e_5 , and e_9 corresponding to the fixed positions 1, 5, and 9, the next three columns consist of eigenvectors $(e_k + e_l)/\sqrt{2}$, and the last three columns consist of eigenvectors $(e_k - e_l)/\sqrt{2}$, where pairs (k, l) correspond to the cycles of order 2 described above.

The latent positions are the rows of

$$XU = \begin{bmatrix} \lambda^{(11)} & 0 & 0 & \lambda^{(12)}/\sqrt{2} & \lambda^{(13)}/\sqrt{2} & 0 & \lambda^{(12)}/\sqrt{2} & \lambda^{(13)}/\sqrt{2} & 0 \\ 0 & \lambda^{(22)} & 0 & \lambda^{(21)}/\sqrt{2} & 0 & \lambda^{(23)}/\sqrt{2} & -\lambda^{(21)}/\sqrt{2} & 0 & \lambda^{(23)}/\sqrt{2} \\ 0 & 0 & \lambda^{(33)} & 0 & \lambda^{(31)}/\sqrt{2} & \lambda^{(32)}/\sqrt{2} & 0 & -\lambda^{(31)}/\sqrt{2} & -\lambda^{(32)}/\sqrt{2} \end{bmatrix}.$$

3 Methods

Two inference objectives arise from the PABM:

1. Cluster membership identification (up to permutation).
2. Parameter estimation (estimating $\lambda^{(kl)}$'s).

Here, we will focus more on (1) and pose possible methods for (2). In our methods, we assume that K , the number of clusters, is known beforehand and does not require estimation.

3.1 Clustering

3.1.1 Using edge probability matrix P

We previously stated one possible set of latent positions that result in the edge probability matrix of a PABM, $P = (XU)I_{pq}(XU)^\top$. If we have (or can estimate) XU directly, then both the clustering and parameter identification problem are trivial since U is orthonormal and fixed for each value of K . However, direct identification or estimation of XU is not possible [3].

If we decompose $P = ZI_{pq}Z^\top$, then $\exists Q \in \mathbb{O}(p, q)$ such that $XU = ZQ$. Even if we start with the exact edge probability matrix, we cannot recover the “original” latent positions XU . Note that unlike in the case of the RDPG, Q is not an orthogonal matrix. If z_i 's are the rows of XU , then $\|z_i - z_j\|^2 \neq \|Qz_i - Qz_j\|^2$, and $\langle z_i, z_j \rangle \neq \langle Qz_i, Qz_j \rangle$. This prevents us from using the properties of XU directly. In particular, if $Q \in \mathbb{O}(n)$, then we could use the fact that $\langle z_i, z_j \rangle = \langle Qz_i, Qz_j \rangle = 0$ if vertices i and j are in different clusters.

We can note from the explicit form of XU that it represents points in \mathbb{R}^{K^2} such that points within each cluster lie on K -dimensional subspaces. Furthermore, the subspaces are orthogonal to each other. Multiplication by $Q \in \mathbb{O}(p, q)$ removes the orthogonality property but retains the property that each cluster is represented by a K -dimensional subspace. Using this property, previous work proposes the use of subspace clustering while acknowledging some of its shortcomings [2] [5].

Theorem 3. Let $P = VDV^\top$ be the spectral decomposition of the edge probability matrix. Let $B = VV^\top$. Then $B_{ij} = 0$ if vertices i and j are of different clusters.

Proof (sketch) By projection, $VV^\top = X(X^\top X)^{-1}X^\top$ where X is defined as in Theorem 2. Since X is block diagonal with each block corresponding to one cluster, $X(X^\top X)^{-1}X^\top$ is also a block diagonal matrix with each block corresponding to a cluster and zeros elsewhere. Therefore, if vertices i and j belong to different clusters, then the ij^{th} element of $X(X^\top X)^{-1}X^\top = VV^\top = B$ is 0.

Algorithm 1: PABM clustering on the edge probability matrix.

Data: Edge probability matrix P , number of clusters K

Result: Cluster assignments $1, \dots, K$

- 1 Compute the spectral decomposition $P = VDV^\top$.
 - 2 Compute the inner product matrix $B = |VV^\top|$, applying $|\cdot|$ entry-wise.
 - 3 Construct graph G using B as edge similarities.
 - 4 Identify the connected components of G and map each to cluster labels $1, \dots, K$.
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3.1.2 Using adjacency matrix A

The adjacency embedding of A approaches latent positions that form P as the number of vertices n increases. More precisely, let $\{\lambda^{(kl)}\}_K \sim \mathcal{F}_K$ for some joint distribution consisting of K underlying clusters \mathcal{F}_K . Then the latent positions $XU \sim \mathcal{G}_K$ for some related joint distribution with K underlying clusters \mathcal{G}_K . Denote Z_n as a sample of size n from \mathcal{G}_K and adjacency matrix A_n as one draw from edge probability matrix $P_n = Z_n I_{pq} Z_n^\top$. Let \hat{Z}_n be the adjacency embedding of A_n with rows $(\hat{z}_i^{(n)})^\top$. Then by Rubin-Delanchy, Cape, Tang, and Priebe [3],

$$\max_{i \in \{1, \dots, n\}} \|Q_n \hat{z}_i^{(n)} - z_i^{(n)}\| = O_P\left(\frac{(\log n)^c}{n^{1/2}}\right)$$

for some $c > 0$ and sequence of $Q_n \in \mathbb{O}(p, q)$. In addition, Rubin-Delanchy et al. produce a central limit theorem result.

Theorem 4. Let $\hat{V}^{(n)} \in \mathbb{R}^{n \times K^2}$ be the matrix of K^2 eigenvectors of A_n corresponding to the $K(K+1)/2$ most positive eigenvalues and $K(K-1)/2$ most negative eigenvalues with rows $(\hat{v}_i^{(n)})^\top$. Let (i, j) correspond to pairs belonging to different clusters. Then for some $c > 0$,

$$\max_{i, j} \|(\hat{v}_i^{(n)})^\top \hat{v}_j^{(n)}\| = O_P\left(\frac{(\log n)^c}{n}\right)$$

In addition, by the central limit theorem, $(\hat{v}_i^{(n)})^\top \hat{v}_j^{(n)}$ converge to a normal distribution centered at 0.

Algorithm 2: PABM clustering on the adjacency matrix.

Data: Adjacency matrix A , number of clusters K

Result: Cluster assignments $1, \dots, K$

- 1 Compute the eigenvectors of A that correspond to the $K(K+1)/2$ most positive eigenvalues and $K(K-1)/2$ most negative eigenvalues. Construct V using these eigenvectors as its columns.
 - 2 Compute $B = |VV^\top|$, applying $|\cdot|$ entry-wise.
 - 3 Construct graph G using B as its similarity matrix.
 - 4 Partition G into K disconnected components (e.g., using edge thresholding or spectral clustering).
 - 5 Map each partition to the cluster labels $1, \dots, K$.
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3.2 Parameter estimation

For any P edge probability matrix for the PABM such that the rows and columns are organized by cluster, the kl^{th} block is an outer product of two vectors, i.e., $P^{(kl)} = \lambda^{(kl)}(\lambda^{(lk)})^\top$. Therefore, given $P^{(kl)}$, λ and $\lambda^{(lk)}$ are solvable exactly (up to multiplication by -1) using singular value decomposition. More specifically, let $P = \sigma^2 uv^\top$ be the singular value decomposition of P . $u \in \mathbb{R}^{n_k}$ and $v \in \mathbb{R}^{n_l}$ are vectors and $\sigma^2 > 0$ is a scalar. Then $\lambda^{(kl)} = \pm \sigma u$ and $\lambda^{(lk)} = \pm \sigma v$.

Algorithm 3: PABM parameter estimation using the edge probability matrix.

Data: Edge probability matrix P , cluster assignments $1, \dots, K$.

Result: PABM parameters $\{\lambda^{(kl)}\}_K$

- 1 Arrange the rows and columns of P by cluster such that each $P^{(kl)}$ block consists of edge probabilities between clusters k and l .
 - 2 **for** $k, l = 1, \dots, K$, $k \geq l$ **do**
 - 3 Compute $P^{(kl)} = (\sigma^{(kl)})^2 u^{(kl)}(v^{(kl)})^\top$, the SVD of the kl^{th} block.
 - 4 Assign $\lambda^{(kl)} \leftarrow \pm \sigma^{(kl)} u^{(kl)}$ and $\lambda^{(lk)} \leftarrow \pm \sigma^{(kl)} v^{(kl)}$.
 - 5 **end**
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A similar method can be applied using \hat{Z} , the adjacency spectral embedding of A .

Algorithm 4: PABM parameter estimation using the adjacency matrix.

Data: Adjacency matrix A , cluster assignments $1, \dots, K$

Result: PABM parameter estimates $\{\hat{\lambda}^{(kl)}\}_K$.

- 1 Assign $p \leftarrow K(K+1)/2$ and $q \leftarrow K(K-1)/2$.
 - 2 Compute \hat{Z} , the adjacency spectral embedding of A using signature (p, q) .
 - 3 Compute $\hat{P} = \hat{Z}I_{pq}\hat{Z}^\top$, the estimate of the edge probability matrix based on the adjacency spectral embedding.
 - 4 Arrange the rows and columns of \hat{P} by cluster such that each $\hat{P}^{(kl)}$ block consists of estimated edge probabilities between clusters k and l .
 - 5 **for** $k, l = 1, \dots, K$, $k \leq l$ **do**
 - 6 Compute $\hat{P}^{(kl)} = U\Sigma V^\top$, the SVD of the kl^{th} block.
 - 7 Assign $u^{(kl)}$ and $v^{(kl)}$ as the first columns of U and V . Assign $\sigma^2 \leftarrow \Sigma_{11}$.
 - 8 Assign $\hat{\lambda}^{(kl)} \leftarrow \pm\sigma^{(kl)}u^{(kl)}$ and $\hat{\lambda}^{(lk)} \leftarrow \pm\sigma^{(kl)}v^{(kl)}$.
 - 9 **end**
-

Theorem 5. Let $\lambda_{n_k}^{(kl)} \sim F_{n_k}$ for $k, l = 1, \dots, K$, and let $\{\hat{\lambda}_{n_k}^{(kl)}\}_K$ be the set of estimates computed by Algorithm 4. Then ... **TODO**

4 Simulated Examples

For these examples, we will set the following parameters:

- $K = 2$
- Mixture parameter $\alpha = .5$
- $\lambda^{(kk)} \stackrel{indep}{\sim} \text{Beta}(2, 1)$
- $\lambda^{(kl)} \stackrel{indep}{\sim} \text{Beta}(1, 2)$ for $k \neq l$

4.1 Clustering

In this part, we will assess Algorithm 2's performance for sample sizes $n = 64, 128, 256, 512, 1024$. For each sample size n , 100 sets of $\lambda^{(kl)}$'s are drawn and for each set of parameters, one adjacency matrix A is drawn and clustered.

We will not consider clustering using the edge probability matrix P since this will always result exact recovery of the original clusters.

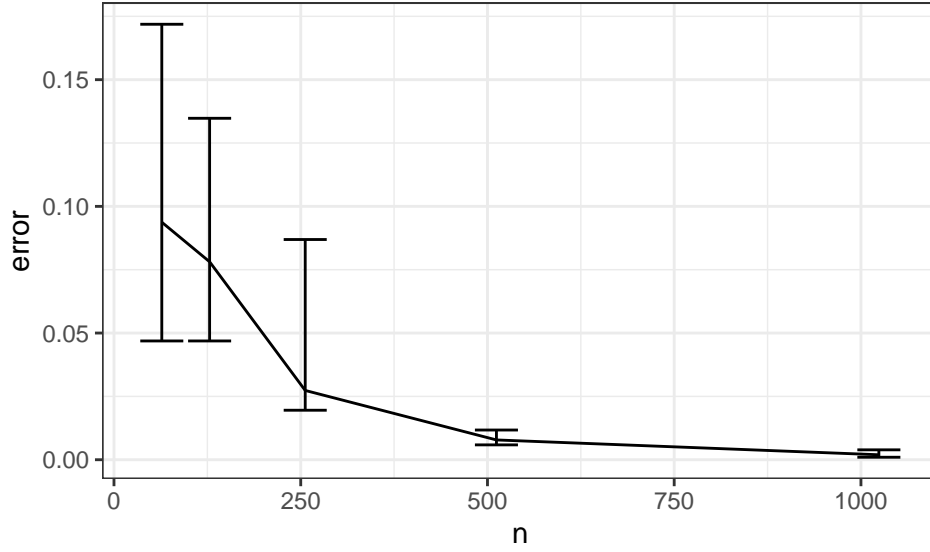


Figure 1: IQR clustering error using Algorithm 1 for sample sizes from 64 to 1024. Simulations were repeated 100 times for each sample size.

We can also examine how the distribution of $(\hat{v}_i)^\top \hat{v}_j$ varies with n :

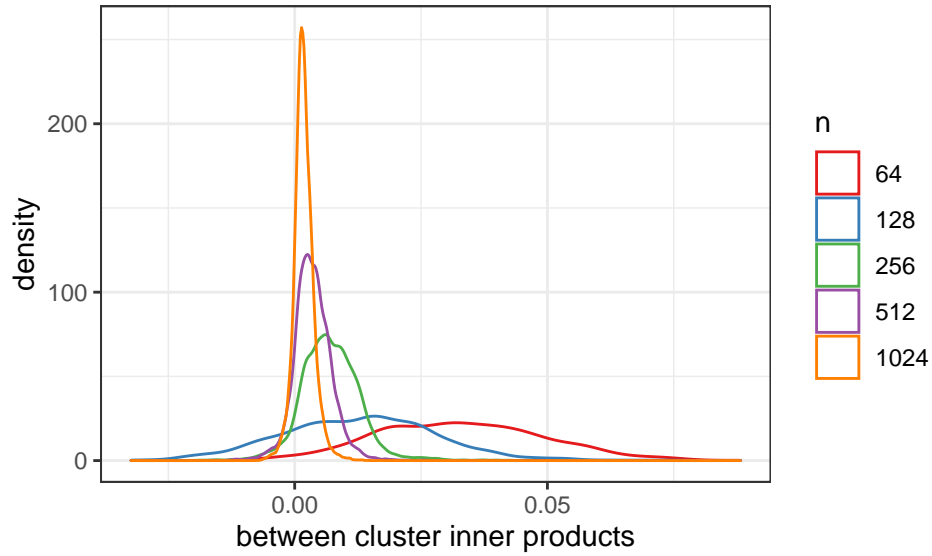


Figure 2: Between-cluster inner products of the eigenvectors of A for varying sample sizes.

4.2 Parameter estimation

Figure 3 shows the medians and interquartile ranges of root mean square errors for Algorithm 4 over 100 simulations using the same parameters as before.

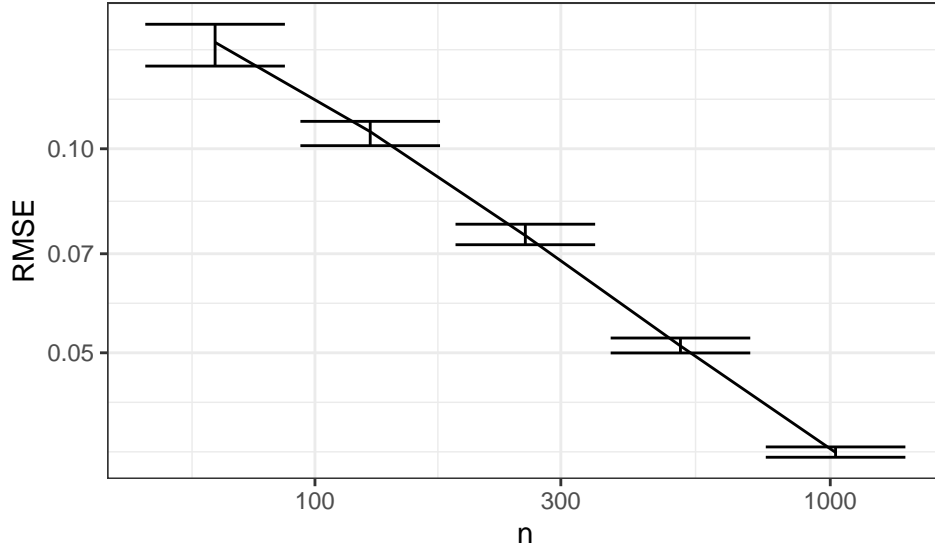


Figure 3: Median and IQR RMSE from Algorithm 4 using sample sizes from 64 to 1024. Simulations were repeated 100 times for each sample size.

References

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