Community Detection Methods for the Generalized Random Dot Product Graph

Dissertation Proposal

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John Koo¹ PhD Candidate Research Committee

Dr. Michael Trosset¹

Dr. Minh Tang²

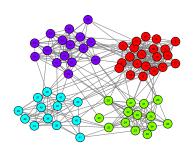
Dr. Julia Fukuyama¹

Dr. Roni Khardon³

Dr. Fangzheng Xie¹

 $^1\mathrm{Department}$ of Statistics, Indiana University $^2\mathrm{Department}$ of Statistics, North Carolina State University $^3\mathrm{Department}$ of Computer Science, Indiana University

Community Detection for Networks



How can we cluster the nodes of a network?

Statistical inference (parametric approach):

- 1. Define a generative model for graph $G \mid z_1,...,z_n, \vec{\theta} \sim P(\vec{z}, \vec{\theta})$.
- 2. Develop a method for obtaining estimators $f(G) = \hat{z}_1,...,\hat{z}_n$.
- 3. Identify asymptotic properties of estimators.

Overview

- 1. Probability Models for Networks
 - a. Block Models and Community Structure
 - b. (Generalized) Random Dot Product Graphs
 - c. Connecting Block Models to the (G)RDPG
- 2. Popularity Adjusted Block Model
 - a. Connecting the PABM to the GRDPG
 - b. Orthogonal Spectral Clustering
 - c. Sparse Subspace Clustering
- Community Detection for the (G)RDPG
 - a. Manifold Clustering
 - b. Manifolds as (G)RDPG Latent Configurations

Probability Models for Networks

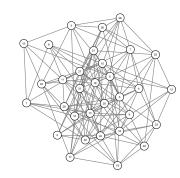
Bernoulli Graphs

Let G = (V, E) be an undirected and unweighted graph with |V| = n. G is described by adjacency matrix A such that $A_{ij} = \begin{cases} 1 & \exists \text{ edge between } i \text{ and } j \\ 0 & \text{else} \end{cases}$ $A_{ji} = A_{ij}$ and $A_{ii} = 0 \ \forall i,j \in [n]$.

 $A \sim \mathsf{BernoulliGraph}(P)$ iff:

- 1. $P \in [0,1]^{n \times n}$ describes edge probabilities between pairs of vertices.
- 2. $A_{ij} \stackrel{\text{ind}}{\sim} \text{Bernoulli}(P_{ij}) \text{ for each } i < j.$

Example 1: If every entry $P_{ij} = \theta$, then $A \sim \text{BernoulliGraph}(P)$ is an Erdos-Renyi graph. For this model, $A_{ij} \stackrel{\text{iid}}{\sim} \text{Bernoulli}(\theta).$



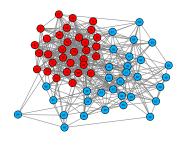
Block Models

Suppose each vertex $v_1,...,v_n$ has hidden labels $z_1,...,z_n\in [K]$, and each P_{ij} depends on labels z_i and z_j .

Example 2: Stochastic Block Model with two communities

Then $A \sim \mathsf{BernoulliGraph}(P)$ is a block model.

- $z_1, ..., z_n \in \{1, 2\}$ • $P_{ij} = \begin{cases} p & z_i = z_j = 1\\ q & z_i = z_j = 2\\ r & z_i \neq z_j \end{cases}$
- To make this an assortative SBM, set $pq>r^2$
- In this example, p=1/2, q=1/4, and r=1/8.



Block Models

Erdos-Renyi Model (1959)

- $P_{ij} = \theta$
- Not a block model

Stochastic Block Model (Lorrain and White, 1971)

- $P_{ij} = \theta_{z_i z_j}$
- K(K+1)/2 parameters θ_{kl}

Degree Corrected Block Model (Karrer and Newman, 2011)

- $P_{ij} = \theta_{z_i z_j} \omega_i \omega_j$
- K(K+1)/2 + n parameters θ_{kl} , ω_i

Popularity Adjusted Block Model (Sengupta and Chen, 2017)

- $P_{ij} = \lambda_{iz_j}\lambda_{jz_i}$
- Kn parameters λ_{ik}

Hierarchy of Block Models

PABM \rightarrow DCBM: $\lambda_{ik} = \sqrt{\theta_{z_i k}} \omega_i$

 $DCBM \rightarrow SBM: \omega_i = 1$

 $\mathsf{SBM} \to \mathsf{Erdos} ext{-Renyi: } \theta_{kl} = \theta$

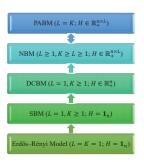


Figure 2: The hierarchy of block models

Majid Noroozi and Marianna Pensky, 2021

(Generalized) Random Dot Product Graph Model

Random Dot Product Graph $A \sim \mathsf{RDPG}(X)$ (Young and Scheinerman, 2007)

- Latent vectors $x_1,...,x_n \in \mathbb{R}^d$ such that $x_i^{\top}x_j \in [0,1]$
- $A \sim \mathsf{BernoulliGraph}(XX^\top)$ where $X = \begin{bmatrix} x_1 & \cdots & x_n \end{bmatrix}^\top$

Generalized Random Dot Product Graph $A \sim \mathsf{GRDPG}_{p,q}(X)$ (Rubin-Delanchy, Cape, Tang, Priebe, 2020)

- Latent vectors $x_1,...,x_n\in\mathbb{R}^{p+q}$ such that $x_i^{\top}I_{p,q}x_j\in[0,1]$ and $I_{p,q}=\mathsf{blockdiag}(I_p,-I_q)$
- $A \sim \mathsf{BernoulliGraph}(XI_{p,q}X^\top)$ where $X = \begin{bmatrix} x_1 & \cdots & x_n \end{bmatrix}^\top$

If latent vectors $X_1,...,X_n \stackrel{\text{iid}}{\sim} F$, then we write $(A,X) \sim \mathsf{RDPG}(F,n)$ or $(A,X) \sim \mathsf{GRDPG}_{p,q}(F,n)$.

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(Generalized) Random Dot Product Graph Model

Recovery/Estimation

Want to estimate X from A, or alternatively, interpoint distances, inner products, or angles.

Adjacency Spectral Embedding

To embed in \mathbb{R}^d ,

- 1. Compute $A \approx \hat{V} \hat{\Lambda} \hat{V}^{\top}$ where $\hat{\Lambda} \in \mathbb{R}^{d \times d}$ and $\hat{V} \in \mathbb{R}^{n \times d}$. For RDPG, use d greatest eigenvalues; for GRDPG, use p most positive and q most negative eigenvalues.
- 2. For RDPG, let $\hat{X}=\hat{V}\hat{\Lambda}^{1/2}$; for GRDPG, let $\hat{X}=\hat{V}|\hat{\Lambda}|^{1/2}$.

RDPG:
$$\max_i \|\hat{X}_i - W_n X_i\| \overset{a.s.}{\to} 0$$
 (Athreya et al., 2018) GRDPG: $\max_i \|\hat{X}_i - Q_n X_i\| \overset{a.s.}{\to} 0$ (Rubin-Delanchy et al., 2020)

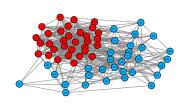
Connecting Block Models to the (G)RDPG Model

All Bernoulli Graphs are RDPG (if P is positive semidefinite) or GRDPG (in general).

Example 2 (cont'd): Assortative SBM $(pq > r^2)$ with K = 2

$$P_{ij} = \begin{cases} p & z_i = z_j = 1\\ q & z_i = z_j = 2\\ r & z_i \neq z_j \end{cases}$$

$$P = \begin{bmatrix} P^{(11)} & P^{(12)} \\ P^{(21)} & P^{(22)} \end{bmatrix} = XX^{\top}$$



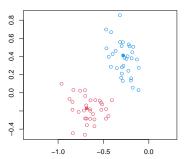
$$X = \begin{bmatrix} \sqrt{p} & 0\\ \vdots & \vdots\\ \sqrt{p} & 0\\ \sqrt{r^2/p} & \sqrt{q - r^2/p}\\ \vdots & \vdots\\ \sqrt{r^2/p} & \sqrt{q - r^2/p} \end{bmatrix}$$

Connecting Block Models to the (G)RDPG Model

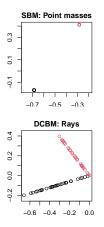
Example 2 (cont'd): If we want to perform community detection,

- 1. Note that A is a RDPG because $P = XX^{\top}$.
- 2. Compute the ASE $A \approx \hat{X}\hat{X}^{\top}$ with $\hat{X} = \hat{V}\hat{\Lambda}^{1/2}$.
- 3. Apply clustering algorithm (e.g., K-means) to \hat{X} , noting that as $n \to \infty$, the ASE approaches point masses.

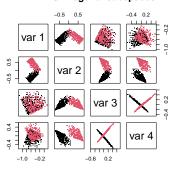
ASE of the adjacency matrix drawn from SBM



Connecting Block Models to the (G)RDPG Model



PABM: Orthogonal subspaces



Popularity Adjusted Block Model

Popularity Adjusted Block Model

Def Popularity Adjusted Block Model (Sengupta and Chen, 2017):

Let each vertex $i \in [n]$ have K popularity parameters $\lambda_{i1},...,\lambda_{iK} \in [0,1]$. Then $A \sim \mathsf{PABM}(P)$ if each $P_{ij} = \lambda_{iz_j}\lambda_{jz_i}$, e.g., if $z_i = k$ and $z_j = l$, $P_{ij} = \lambda_{il}\lambda_{jk}$.

Lemma (Noroozi, Rimal, and Pensky, 2020):

A is sampled from a PABM if P can be described as:

- 1. Let each $P^{(kl)}$ denote the $n_k \times n_l$ matrix of edge probabilities between communities k and l.
- 2. Organize popularity parameters as vectors $\lambda^{(kl)} \in \mathbb{R}^{n_k}$ such that $\lambda_i^{(kl)} = \lambda_{k_i l}$ is the popularity parameter of the i^{th} vertex of community k towards community l.
- 3. Each block can be decomposed as $P^{(kl)} = \lambda^{(kl)} (\lambda^{(lk)})^{\top}$.

Notation: $A \sim \mathsf{PABM}(\{\lambda^{(kl)}\}_K)$.

Connecting the PABM to the GRDPG

Theorem (KTT): $A \sim \mathsf{PABM}(\{\lambda^{(kl)}\}_K)$ is equivalent to $A \sim \mathsf{GRDPG}_{p,q}(XU)$ with

- p = K(K+1)/2, q = K(K-1)/2
- $U \in \mathbb{O}(K^2)$
- $X \in \mathbb{R}^{n \times K^2}$ is block diagonal and composed of $\{\lambda^{(kl)}\}_K$ with each block corresponding to a community.

$$X = \begin{bmatrix} \Lambda^{(1)} & \cdots & 0 \\ 0 & \ddots & 0 \\ 0 & \cdots & \Lambda^{(K)} \end{bmatrix} \in \mathbb{R}^{n \times K^2}$$

$$\Lambda^{(k)} = \begin{bmatrix} \lambda^{(k1)} & \cdots & \lambda^{(kK)} \end{bmatrix} \in \mathbb{R}^{n_k \times K}$$

Connecting the PABM to the GRDPG

$$X = \begin{bmatrix} \Lambda^{(1)} & \cdots & 0 \\ 0 & \ddots & 0 \\ 0 & \cdots & \Lambda^{(K)} \end{bmatrix} \qquad U \in \mathbb{O}(K^2)$$

$$A \sim \mathsf{PABM}(\{\lambda^{(kl)}\}_K) \iff A \sim \mathsf{GRDPG}_{p,q}(XU)$$

Remark 1 (orthogonality of subspaces): If y_i^{\top} and y_j^{\top} are two rows of XU corresponding to different communities, then $y_i^{\top}y_j=0$.

Remark 2 (non-uniqueness of the latent configuration): If $A \sim \mathsf{GRDPG}_{p,q}(Y)$, then $A \sim \mathsf{GRDPG}_{p,q}(YQ)$ for any Q in the indefinite orthogonal group with signature p,q.

Remark 3: Communities correspond to subspaces even with linear transformation $Q\in \mathbb{O}(p,q)$, but this may break the orthogonality property.

Orthogonal Spectral Clustering

Theorem (KTT): If $P = V\Lambda V^{\top}$ and $B = nVV^{\top}$, then $B_{ij} = 0$ if $z_i \neq z_j$.

Algorithm: Orthogonal Spectral Clustering:

- 1. Let V be the eigenvectors of A corresponding to the K(K+1)/2 most positive and K(K-1)/2 most negative eigenvalues.
- 2. Compute $B = |nVV^{\top}|$ applying $|\cdot|$ entry-wise.
- 3. Construct graph G using B as its similarity matrix.
- 4. Partition G into K disconnected subgraphs.

Theorem (KTT): Let \hat{B}_n with entries $\hat{B}_n^{(ij)}$ be the affinity matrix from OSC. Then \forall pairs (i,j) belonging to different communities and sparsity factor satisfying $n\rho_n = \omega\{(\log n)^{4c}\}$,

$$\max_{i,j} \hat{B}_n^{(ij)} = O_P\left(\frac{(\log n)^c}{\sqrt{n\rho_n}}\right)$$

Sparse Subspace Clustering

Corollary: The ASE of $A \sim \mathsf{PABM}(\{\lambda^{(kl)}\}_K)$ lies near a collection of K-dimensional subspaces in K^2 dimensions.

Algorithm: Sparse Subspace Clustering (Elhamifar & Vidal, 2009):

1. Solve n optimization problems $c_i = \arg\min_c \|c\|_1$ subject to $x_i = X^{\top}c$ and $c^{(i)} = 0$. This is typically performed via LASSO:

$$c_i = \arg\min \frac{1}{2} ||x_i - X_{-i}^{\top} c||_2^2 + \lambda ||c||_1$$

- 2. Compile solutions $C = \begin{bmatrix} c_1 & \cdots & c_n \end{bmatrix}$.
- 3. Construct affinity matrix $B = |C| + |C^{\top}|$.

Sparse Subspace Clustering

Noroozi et al. observed that the rank of P is K^2 and the columns of P belonging to each community has rank K to justify SSC for the PABM.

$$c_i = \arg\min_{c} \|c\|_1$$
 subject to $A_{\cdot,i} = Ac$ and $c^{(i)} = 0$

They were able to show that this obeys SDP if we replace A with P.

GRDPG-based approach: Apply SSC to the ASE of ${\cal A}.$

Stronger result: Apply SSC to the eigenvectors of ${\cal A}.$

$$c_i = \arg\min_c \|c\|_1$$
 subject to $\hat{v}_i = \hat{V}^{ op}c$ and $c^{(i)} = 0$
$$A \approx \hat{V}\hat{\Lambda}\hat{V}^{ op}$$

Sparse Subspace Clustering

Theorem (KTT):

Let

- P_n describe the edge probability matrix of the PABM with n vertices, and $A_n \sim \text{BernoulliGraph}(P_n)$;
- \hat{V}_n be the matrix of eigenvectors of A_n corresponding to the K(K+1)/2 most positive and K(K-1)/2 most negative eigenvalues.

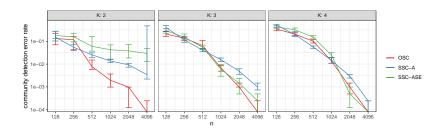
Then

• For some $\lambda>0$ and $N<\infty$, $\sqrt{n}\hat{V}_n$ obeys the Subspace Detection Property with probability 1 when n>N.

Remarks:

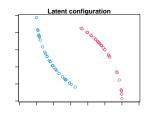
- For large n, we can identify λ for SDP (Wang and Xu, 2016).
- SDP does not guarantee community detection.

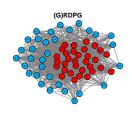
Simulation Study

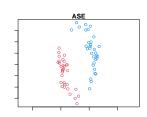


General Community Detection for the (G)RDPG

Recovery from the Adjacency Matrix







Generative Model

Let $(A,X) \sim \mathsf{GRDPG}_{p,q}(F,n)$ as follows:

- 1. Define functions $\gamma_1, ..., \gamma_K$ such that each $\gamma_k : [0, 1]^r \mapsto \mathbb{R}^d$ and $\gamma_k(t) \neq \gamma_l(t)$ when $k \neq l$.
- 2. Sample labels $Z_1,...,Z_n \stackrel{\mathsf{iid}}{\sim} \mathsf{Categorical}(\pi_1,...,\pi_K)$.
- 3. Sample $T_1, ..., T_n \stackrel{\text{iid}}{\sim} D$ with support $[0, 1]^r$.
- 4. Set latent positions $X_i = \gamma_{Z_i}(T_i)$ and $X = \begin{bmatrix} X_1 & \cdots & X_n \end{bmatrix}^{\top}$.
- 5. $A \sim \mathsf{BernoulliGraph}(XI_{p,q}X^\top)$

Examples:

- 1. r=1 and each γ_k is a point mass \Longrightarrow SBM
- 2. r=1 and the range of each γ_k is a segment from the origin to point y_k with $\|y_k\| \leq 1 \implies \mathsf{DCBM}$
- 3. r=K and the range of each γ_k is the hyperplane of coordinates $x_{K(k-1)+1}$ to $x_{kK} \Longrightarrow \mathsf{PABM}$

Community Detection

Recall that the ASE approximates the true latent positions:

$$\max_{i} \|\hat{X}_{i} - Q_{n}X_{i}\| \stackrel{a.s.}{\to} 0$$

This suggests a general approach to community detection:

Given A, K, and d (or p and q),

- 1. Use ASE to approximate the latent configuration.
- 2. Use an appropriate clustering algorithm for the latent configuration.

Parallel Segments

Example 3: Let $U_1,...,U_{n_1},U_{n_1+1},...,U_n \stackrel{\text{iid}}{\sim} \text{Uniform}(0,\theta)$, $\gamma_1(t)=(t,0)$, and $\gamma_2(t)=(t,a)$. $X_i=\gamma_1(U_i)$ for $i\leq n_1$ and $X_j=\gamma_2(U_j)$ for $n_1+1\leq j\leq n$. If we observe $X_1,...,X_{n_1},X_{n_1+1},...,X_n$, what approach will allow us to group the observations by segment?

Then for any $a \in (0,1)$, $\delta \in (0,1)$, we can find $N(a,\delta) < \infty$ such that when $\min_k n_k \geq N$, with probability at least $1-\delta$,

- 1. Single linkage clustering entails perfect community detection.
- 2. Any ϵ -neighborhood graph with $\epsilon \leq a$ will consist of at least K disjoint subgraphs such that no subgraph contains members of two different communities.

Noisy Parallel Segments and One-Dimensional Manifolds

Example 4: Starting with the parallel segments as before, suppose instead of observing $X_1,...,X_n$, we have noisy observations $X_1+\xi_1,...,X_n+\xi_n$ such that $\max_i \|\xi_i\|=\xi \leq a/3$.



Then we can derive similar statements as in Example 3.

This also holds for noisy points sampled uniformly on one-dimensional manifolds such that the manifolds are distance at least a apart.

Since the ASE of a RDPG generated from points on these segments/curves will reconstruct the original segments/curves with noise, we can apply this to the RDPG (if sufficient n).

Future Work

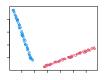
- 1. Derive formal statements showing that the ASE of a random graph generated by these latent configurations produces the correct conditions for community detection.
- 2. Extend results to non-uniform distributions.
- 3. Extend results to multidimensional manifolds.
- 4. Relax condition for the minimum distance between manifolds.
- 5. Extend results to the GRDPG.

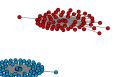
Thank you

Additional Slides

Subspace Detection Property

If X obeys the Subspace Detection Property, then B is sparse such that $B_{ij}=0$ for each x_i and x_j belonging to different subspaces.





Theorem (Wang and Xu, 2016): If data matrix X consists of points lying close to low-dimensional subspaces such that:

- 1. Each point's distance to its subspace is sufficiently small.
- 2. The points corresponding to each subspace cover a sufficient amount of that subspace.
- 3. The cosine of the angles between pairs of subspaces is sufficiently small.

Then X obeys SDP.

Parameter Estimation

- 1. Let $A^{(kl)}$ be the block of edges between communities k and l.
- 2. For each $k, l \in [K]$, do:
 - i. Compute the SVD $A^{(kl)} = U\Sigma V^{\top}$.
 - ii. Assign $u^{(kl)}$ and $v^{(kl)}$ as the first columns of U and V. Assign $\sigma^{(kl)} \leftarrow \Sigma_{11}^{1/2}$.
 - iii. Assign $\hat{\lambda}^{(k\bar{l})} \leftarrow \pm \sigma^{(kl)} u^{(kl)}$ and $\hat{\lambda}^{(kl)} \leftarrow \pm \sigma^{(kl)} v^{(kl)}$.

Theorem (KTT):

$$\max_{k,l} \|\hat{\lambda}^{(kl)} - \lambda^{(kl)}\| = O_P\left(\frac{(\log n_k)^c}{\sqrt{n_k}}\right)$$

Indefinite Orthogonal Group

$$\mathbb{O}(p,q) = \{ Q : Q I_{p,q} Q^{\top} = I_{p,q} \}$$

- $Q^{\top}Q \neq I$
- If $A \sim \mathsf{GRDPG}_{p,q}(X)$, then $A \sim \mathsf{GRDPG}_{p,q}(XQ)$
- $(Qx)^{\top}(Qy) = x^{\top}Q^{\top}Qy \neq x^{\top}y$
- $||Q|| \neq 1 \implies ||Qx Qy|| \neq ||x y||$

Non-Spectral Community Detection for Block Models

Likelihood

$$L = \prod_{i < j} \prod_{k,l}^{K} \left(p_{k,l,i,j}^{A_{ij}} (1 - p_{k,l,i,j})^{1 - A_{ij}} \right)^{z_{ik} z_{jl}}$$

Example: DCBM $(p_{k,l,i,j} = \theta_{kl}\omega_i\omega_j)$

$$L = \prod_{i < j} \prod_{k,l}^{K} \left((\theta_{kl} \omega_i \omega_j)^{A_{ij}} (1 - \theta_{kl} \omega_i \omega_j)^{1 - A_{ij}} \right)^{z_{ik} z_{jl}}$$

- ML method for community detection: $\hat{\vec{z}} = \arg\max_{\vec{z}} L$
- NP-complete
 - Expectation-Maximization
 - Bayesian methods
 - Spectral methods

Expectation Maximization for the PABM

Full data log-likelihood

$$\log L = \sum_{i < j} \sum_{k,l} z_{ik} z_{jl} (A_{ij} \log \lambda_{il} \lambda_{jk} + (1 - A_{ij}) \log(1 - \lambda_{il} \lambda_{jk}))$$
$$+ \sum_{i} \sum_{k} z_{ik} \log \pi_{k}$$

E-step

- $\gamma_{ik} = P(Z_i = k \mid \{\pi_l\}, \{\lambda_{jl}\})$
- $\log \gamma_{ik} \propto \log \pi_k + \sum_{j \neq i} \sum_l \pi_{jl} (A_{ij} \log \lambda_{il} \lambda_{jk} + (1 A_{ij}) \log(1 \lambda_{il} \lambda_{jk}))$

M-step

- $\pi_k = \frac{1}{n} \sum_i \gamma_{ik}$
- $\{\lambda_{ik}\} = \arg\max_{\{\lambda_{ik}\}} E_Z[\log L]$

MCMC Sampling for the PABM

Priors:

- $Z_i \stackrel{\text{iid}}{\sim} \mathsf{Categorical}(\pi_1, ..., \pi_K)$
- $\lambda_{ik} \stackrel{\text{ind}}{\sim} \mathsf{Beta}(a_{ik}, b_{ik})$

Full joint distribution:

$$\log p = constant$$

$$+ \sum_{i < j} \sum_{k} \sum_{l} z_{ik} z_{jl} (A_{ij} \log \lambda_{il} \lambda_{jk} + (1 - A_{ij}) \log(1 - \lambda_{il} \lambda_{jk}))$$

$$+ \sum_{k} \sum_{i} z_{ik} \log \pi_{k}$$

$$+ \sum_{i} \sum_{k} (a_{ik} - 1) \log \lambda_{ik} + (b_{ik} - 1) \log(1 - \lambda_{ik})$$

Variational Inference for the PABM

Mean Field Variational Inference

- Minimize $d_{KL}(p||q)$
 - ullet p is the joint distribution
 - q is a density of some form
- Restrict $q(\vec{z}, \{\lambda_{ik}\}) = \Big(\prod_i q_{z_i}(z_i)\Big) \Big(\prod_{i,k} q_{\lambda_{ik}}(\lambda_{ik})\Big)$
- Iterative solution: $q_{\theta_i}^{(t+1)} \propto \exp(E_{\theta_{-i}^{(t)}}[\log p])$
- Approximate solution for the PABM
 - $Z_i \mid \{a'_{ik}\}, \{b'_{ik}\} \sim \mathsf{Categorical}(\pi'_1, ..., \pi'_K)$
 - $\bullet \ \, \lambda_{ik} \mid \{a'_{-i,-k}\}, \{b'_{-i,-k}\}, \{\pi'_k\} \sim \mathsf{Beta}(a'_{ik}, b'_{ik})$
 - Iteratively update $\{\pi_K'\}, \{a_{ik}'\}, \{b_{ik}'\}$ until convergence