Manifold Clustering in the Setting of Generalized Random Dot Product Graphs

SDSS Lightning Presentation

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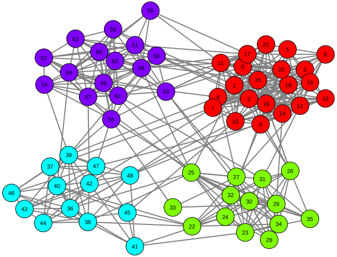
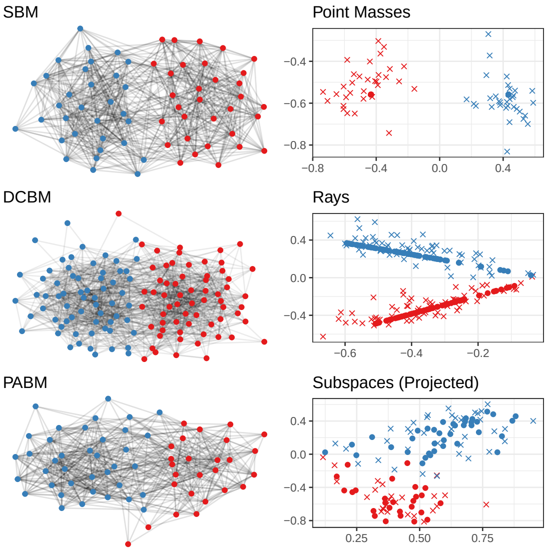


How might we cluster the nodes of a network?

Connecting Block Models to the GRDPG

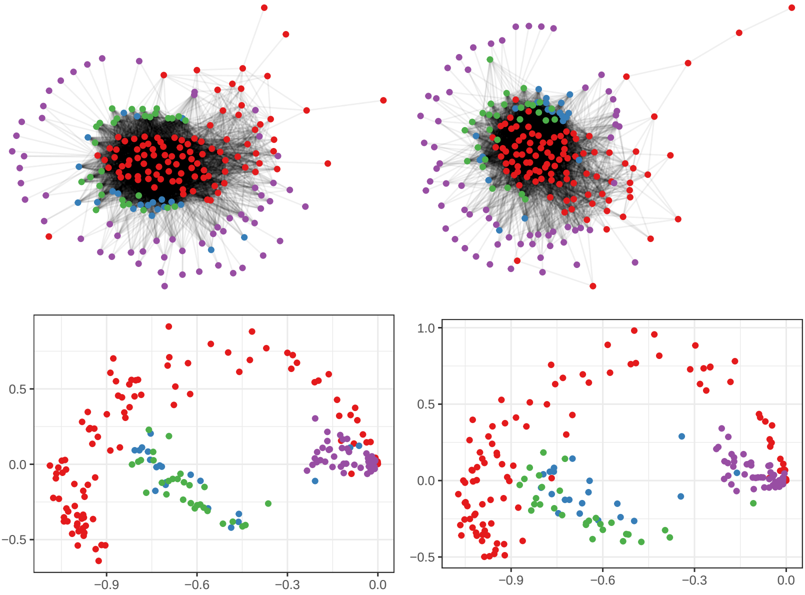


- K-means clustering
- Gaussian mixture models

- K-means with cosine similarity
- GMM on angles

- Orthogonal Spectral Clustering
- Sparse Subspace Clustering

Nonlinear Communty Structure



Manifold Block Model

Let $p, q \geq 0$, $d = p + q \geq 1$, $1 \leq r < d$, $K \geq 2$, and $n > K$ be integers. Define manifolds $\mathcal{M}_1, ..., \mathcal{M}_K \in \mathcal{X}$ for $\mathcal{X} = \{x, y \in \mathbb{R}^d : x^\top I_{p,q} y \in [0, 1]\}$ each by continuous function $g_k : [0, 1]^r \to \mathcal{X}$. Define probability distribution F with support $[0, 1]^r$. Then the following mixture model is a *manifold block model*:

1. Draw labels $z_1, ..., z_n \overset{\text{iid}}{\sim}$ Categorical$(\alpha_1, ..., \alpha_K)$.
2. Draw latent vectors by first taking $t_1, ..., t_n \overset{\text{iid}}{\sim} F$ and then computing each $x_i = g_{z_i}(t_i)$.
3. Compile the latent vectors into data matrix $X = [x_1 \mid \cdots \mid x_n]^\top$ and define the adjacency matrix as $A \sim \text{GRDPG}_{p,q}(X)$.

Manifold Block Model

1. $z_1, \ldots, z_n \overset{\text{iid}}{\sim} \text{Categorical}(1/2, 1/2)$
2. $t_1, \ldots, t_n \overset{\text{iid}}{\sim} \text{Uniform}(0, 1)$
3. $x_i = g_{z_i}(t_i)$
   - $g_1(t) = [t^2, 2t(1-t)]^\top$
   - $g_2(t) = [2t(1-t), (1-t)^2]^\top$
4. $A \sim \text{GRDPG}_{2,0}(X)$

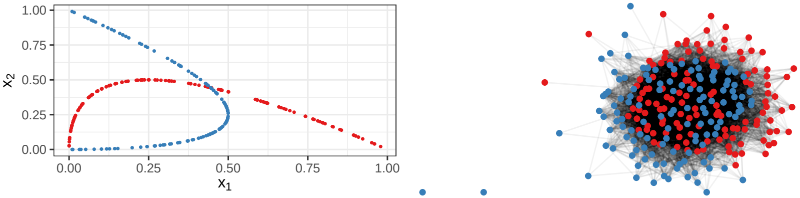


Figure 1: Latent vectors on intersecting curves (left), along with an RDPG drawn from this configuration (center) and its ASE (right).

K-Curves Clustering

Algorithm 1: K-curves clustering.

Data: Adjacency matrix A, number of communities K, embedding dimensions p, q, stopping criterion ϵ

Result: Community assignments $1, \ldots, K$, curves $g_1, \ldots, g_K$

Compute X, the ASE of A using the p most positive and q most negative eigenvalues and their corresponding eigenvectors.

Initialize community labels $z_1, \ldots, z_n$.

repeat

  for $k = 1, \ldots, K$ **do**

    Define X_k as the rows of X for which $z_i = k$.

    Fit curve g_k and positions t_{k_i} to X_k by minimizing $\sum_{k_i} \|x_{k_i} - g_k(t_{k_i})\|^2$.

  end

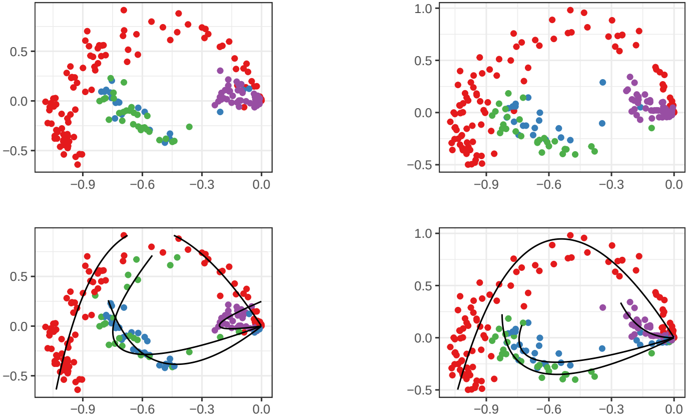
  for $k = 1, \ldots, K$ **do**

    Assign $z_i \leftarrow \arg\min_\ell \|x_i - g_\ell(t_i)\|^2$.

  end

until *the change in* $\sum_k \sum_{i \in C_k} \|x_i - g_k(t_i)\|^2$ *is less than* ϵ

Example


0.5
0.0
−0.5
−0.9
−0.6
−0.3
0.0
1.0
0.5
0.0
−0.5
−0.9
−0.6
−0.3
0.0
0.5
0.0
−0.5
−0.9
−0.6
−0.3
0.0
1.0
0.5
0.0
−0.5
−0.9
−0.6
−0.3
0.0

Asymptotic Results

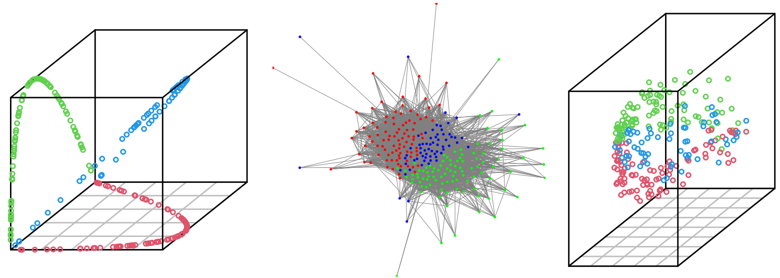
Theorem. Let an MBM be such that the manifolds are described by functions $g_1(t), ..., g_K(t)$ which are polynomial curves of order R. Define the loss of K-curves clustering as:

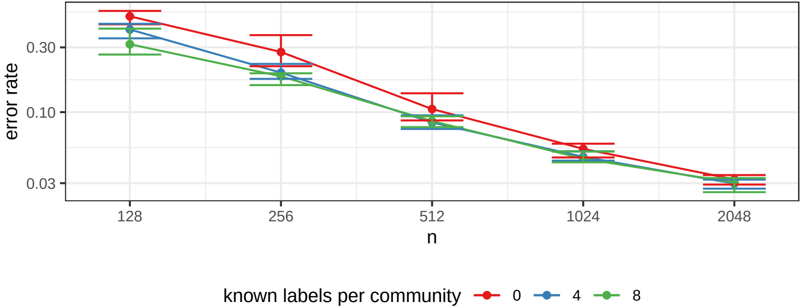
$$L(\hat{z}_1, ..., \hat{z}_n, \hat{g}_1, ..., \hat{g}_K; A) = \sum_k \sum_{i:\hat{z}_i = k} \|\hat{x}_i - \hat{g}_k(t_i)\|^2,$$

where $\hat{x}_i$ are the embedding vectors of A. Suppose that for each community k, we have labels for at least $R+1$ vertices. Then as $n \to \infty$, K-curves clustering outputs estimates such that

$$L(\hat{z}_1, ..., \hat{z}_n, \hat{g}_1, ..., \hat{g}_K; A) \xrightarrow{p} 0.$$

Simulation




error rate
0.30
0.10
0.03
128
256
512
1024
2048
n
known labels per community
0
4
8

Thank you!

Code and drafts available at
https://github.com/johneverettkoo/manifold-block-models