# Manifold Clustering in the Generalized Random Dot Product Graph

John Koo Department of YYY, University of XXX

May 4, 2022

#### Abstract

The text of your abstract. 200 or fewer words.

Keywords: block models, community detection, coordinate descent, latent structure models, manifold clustering, random dot product graph

### 1 Introduction

We define a *Bernoulli graph* as a random graph model for which edge probabilities are contained in an edge probability matrix  $P \in [0,1]^{n \times n}$ , and an edge occurs between vertices i and j with probability  $P_{ij}$ . Common random graph models then impose structure on P, based on various assumptions about the way in which the data are generated, or to allow P to be estimated. One example is the Erdös-Rényi model, in which all edge probabilities are fixed, i.e.,  $P_{ij} = p$ .

One common analysis task for graph and network data is community detection, which assumes that each vertex of a graph has a hidden community label. The goal of the analysis is then to retrieve these labels. In order to perform this analysis as a statistical inference task is to define a probability model with inherent community structure. We call such models block models: First, each vertex is assigned a label  $z_1, ..., z_n \in \{1, 2, ..., K\}$  where  $K \ll n$ . Then each edge probability  $P_{ij}$  is said to depend on the labels  $z_i$  and  $z_j$ , possibly along with some other parameters. For example, the stochastic block model (SBM) sets a fixed edge probability for each pair of communities, i.e.,  $P_{ij} = \omega_{z_i,z_j}$ . The degree-corrected block model (DCBM) assigns an additional parameter  $\theta_i$  to each vertex by which edge probabilities are scaled, i.e.,  $P_{ij} = \theta_i \theta_j \omega_{z_i,z_j}$ . The popularity adjusted block model (PABM) assigns K parameters to each vertex  $\lambda_{i1}, \lambda_{i2}, ..., \lambda_{iK}$  that describe that vertex's affinity toward each community; the edge probability between vertices i and j is then defined as the product of vertex i's affinity toward vertex j's community and vertex j's affinity toward vertex i's community, i.e.,  $P_{ij} = \lambda_{iz_i} \lambda_{jz_i}$ .

The three block model types, as well as the Erdös-Rényi model, impose structure on P, including on the rank of P. P has rank 1 for the Erdös-Rényi model, rank K for the SBM and DCBM, and rank  $K^2$  for the PABM. This provides the intuition behind another family of Bernoulli graphs called the random dot product graph (RDPG) and generalized random dot product graph (GRDPG). In the RDPG, each vertex has a corresponding latent vector in d-dimensional Euclidean space, where d is the rank of P and P is positive semidefinite. Then the edge probability between each pair of vertices is defined as the inner product between the corresponding latent vectors, i.e.,  $P_{ij} = x_i^{\top} x_j$ . If the latent vectors are collected in a data matrix  $X = \begin{bmatrix} x_1 & \cdots & x_n \end{bmatrix}^{\top}$ , then the edge probability matrix for the RDPG is

 $P = XX^{\top}$ . Similarly, the edge probability between each pair of vertices for the GRDPG is defined as the indefinite inner product between the corresponding latent vectors, i.e.,  $P_{ij} = x_i^{\top} I_{p,q} x_j$ , where  $I_{p,q} = \text{blockdiag}(I_p, -I_q)$  and p + q = d. Then the edge probability matrix for the GRDPG is  $P = XI_{p,q}X^{\top}$ . This allows for a model similar to the RDPG for non-positive semidefinite P. While the RDPG and GRDPG do not necessarily have community structure, it has been shown that block models are specific cases of the RDPG or GRDPG in which latent vectors are organized by community. This includes the SBM, in which communities correspond to point masses, DCBM, in which communities correspond to line segments, and PABM, in which communities correspond to orthogonal subspaces. In this work, we extend this idea to communities organized into more general latent structures. In particular, we assume that each community corresponds to a manifold in the latent space.

# 2 Generalized Random Dot Product Graphs with Community Structure

All Bernoulli graphs are generalized random dot product graphs. Whether this is useful for inference depends on the structure of the latent space. In the case of the Erdös-Rényi model, SBM, DCBM, and PABM, the latent structure is linear, and the linearity can be exploited for community detection and parameter estimation. In this section, we discuss general, often nonlinear latent structure models, focusing on those with community structure.

To motivate this, consider a generalization of the Erdös-Rényi model. Recall that when viewed as an RDPG, the latent space of an Erdös-Rényi model consists of one point in Euclidean space. In the following example, instead of fixing the edge probability, it is sampled from a distribution in such a way that when viewed as an RDPG, the latent space consists of a curve.

**Example 1** (Hierarchical Erdös-Rényi model). In the Erdös-Rényi model, the edge probability matrix has a fixed value  $[P_{ij}] \equiv p \in [0,1]$ . Suppose instead that each  $P_{ij}$  is drawn from a distribution with density  $f(p) = \frac{1}{\frac{\pi}{2}-1} \left(\frac{1}{\sqrt{1-p^2}}-1\right)$ .

Then it can be shown that this model is equivalent to a random dot product graph with a two dimensional latent space in which latent vectors are sampled uniformly along

the curve  $g(t) = \begin{bmatrix} \cos(\frac{\pi}{2}t) & \sin(\frac{\pi}{2}t) \end{bmatrix}^{\top}, 0 \le t \le 1.$ 

**Definition 1** (Manifold block model). Let  $p, q \ge 0$ ,  $d = p + q \ge 1$ ,  $K \ge 1$ , and  $n \ge 1$  be integers. If there are manifolds  $\mathcal{M}_1, ..., \mathcal{M}_K \subset \mathcal{X}$  for  $\mathcal{X} = \{x, y \in \mathbb{R}^d : x^\top I_{p,q} y \in [0, 1]\}$ , and  $X = \begin{bmatrix} x_1 & \cdots & x_n \end{bmatrix}^\top$  such that each  $x_i \in \mathcal{M}_k$  for some  $k \in [K]$ , then  $A \sim \text{GRDPG}_{p,q}(X; \rho_n)$  is a manifold block model.

In practice, we often define each manifold  $\mathcal{M}_k$  by a continuous function  $g_k : [0,1]^r \to \mathcal{X}$ , where  $1 \leq r < d$  is the dimensionality of manifold  $\mathcal{M}_k$ . To complete the probability model, we define a probability distribution F with support  $[0,1]^r$  and draw the community memberships from a multinomial distribution.

The full mixture model can be described as follows:

- 1. Draw labels  $z_1, ..., z_n \stackrel{\text{iid}}{\sim} \text{Multinomial}(\alpha_1, ..., \alpha_K)$ .
- 2. Draw latent vectors by first drawing each  $t_1, ..., t_n \stackrel{\text{iid}}{\sim} F$  and then computing each  $x_i = g_{z_i}(t_i)$ .
- 3. Let  $X = \begin{bmatrix} x_1 & \cdots & x_n \end{bmatrix}^{\mathsf{T}}$ , and draw  $A \sim \mathrm{RDPG}(X)$  or  $A \sim \mathrm{GRDPG}_{p,q}(X)$ .

**Example 2.** Let p=2, q=0, K=2, and r=1. Define two one-dimensional manifolds by  $f_1(t) = \left[\cos(\frac{\pi}{3}t) \sin(\frac{\pi}{3}t)\right]^{\top}$  and  $f_2(t) = \left[1-\cos(\frac{\pi}{3}t) \ 1-\sin(\frac{\pi}{3}t)\right]^{\top}$ . Draw  $t_1,...,t_n \stackrel{\text{iid}}{\sim}$  Uniform(0,1) and  $z_1,...,z_n \stackrel{\text{iid}}{\sim}$  Multinomial( $\frac{1}{2},\frac{1}{2}$ ), and compute latent vectors  $x_i = f_{z_i}(t_i)$ , which are collected in data matrix  $X = \begin{bmatrix} x_1 & \cdots & x_n \end{bmatrix}^{\top}$ . Finally, let  $A \sim \text{RDPG}(X)$ . Fig 1 shows the latent configuration drawn from this latent distribution, a random dot product graph drawn from the latent configuration, and the adjacency spectral embedding of the graph.

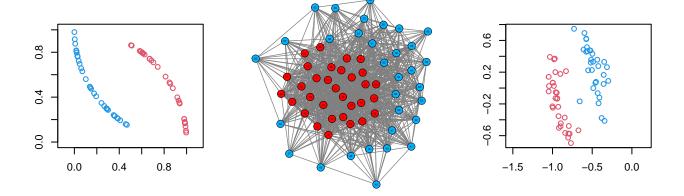


Figure 1: Manifold block model described in Example 1. The latent configuration is on the left, and a random dot product graph drawn from the latent configuration is on the middle, and the ASE is on the right.

### 3 Methods

We provide two approaches to community detection for the manifold block model. First, we consider the case in which communities correspond to manifolds in the latent space that do not intersect and are separated by some finite distance. In this scenario, we use the convergence of the ASE to show that single linkage clustering on the latent space produces a clustering such that the total number of misclustered vertices goes to zero, with high probability.

Next, we consider the case in which communities correspond to one-dimensional manifolds in the latent space and may or may not intersect. In this scenario, we propose an alternating coordinate descent algorithm that alternates between estimating the structure of the manifolds and the community labels, which we call K-curves clustering. We again use the convergence of the ASE to show that under certain conditions, K-curves clustering produces a clustering such that the proportion of misclustered vertices goes to zero, with high probability.

#### 3.1 Nonintersecting Manifolds

In this section, we consider the following scenario: Suppose that each community is represented by a closed manifold  $\mathcal{M}_k$ ,  $k \in \{1, ..., K\}$  in the latent space of a RDPG or GDRPG. Define  $\delta = \min_{k \neq \ell} \min_{x \in \mathcal{M}_k, y \in \mathcal{M}_\ell} ||x - y||$ , the minimum distance between two manifolds. We assume that  $\delta > 0$ , i.e., the manifolds do not intersect.

In the noiseless setting, if the subsample on each manifold is sufficiently dense, it is possible to construct for each manifold an  $\eta_k$ -neighborhood graph for each manifold for some  $\eta_k > 0$  such that the graph is connected. Then if  $\max_k \eta_k = \eta < \delta$ , an  $\eta$ -neighborhood graph for the entire sample will consist of K disconnected subgraphs that map onto each manifold. Equivalently, we can apply single-linkage clustering. The remainder of this section explores under which conditions these criteria are met for the latent configuration, in which latent vectors lie exactly on manifolds, as well as the ASE, which introduces noise.

#### Algorithm 1: ASE clustering for nonintersecting communities.

**Data:** Adjacency matrix A, number of communities K, embedding dimensions p and q.

**Result:** Community assignments  $z_1, ..., z_n \in \{1, ..., K\}$ .

- 1 Compute  $\hat{X}$ , the ASE of A using the p most positive and q most negative eigenvalues and their corresponding eigenvectors.
- **2** Apply single linkage clustering with K communities on  $\hat{X}$ .

Let  $F_k$  be a probability distribution with support  $\mathcal{M}_k$ . Then we define a mixture model as follows:

- 1. Draw labels  $z_1,...,z_n \stackrel{\text{iid}}{\sim} \text{Multinomial}(\alpha_1,...,\alpha_K)$ .
- 2. Draw latent vectors each as  $x_i \stackrel{\text{ind}}{\sim} F_{z_i}$  for distributions  $F_1, ..., F_K$  with respective supports  $\mathcal{M}_1, ..., \mathcal{M}_K$ .
- 3. Let  $X = \begin{bmatrix} x_1 & \cdots & x_n \end{bmatrix}^{\mathsf{T}}$ , and draw  $A \sim \mathrm{RDPG}(X)$  or  $A \sim \mathrm{GRDPG}_{p,q}(X)$ .

Note that here, we redefine the model to ignore  $g_1, ..., g_K$ , the parameterizations of each manifold. Instead, we sample points directly on the manifolds themselves. We will return to the parameterizations in Section 3.2.

**Theorem 1** (Community detection for nonintersecting manifolds without noise). Let  $x_1, ..., x_n$  be points sampled on K manifolds  $\mathcal{M}_1, ..., \mathcal{M}_K$ . Suppose  $\delta = \min_{k \neq \ell} \min_{x_i \in \mathcal{M}_k, x_j \in \mathcal{M}_\ell} ||x_i - x_j|| > 0$ . Define  $A_n$  as the event that for a  $\eta$ -neighborhood graph constructed from the sample  $x_1, ..., x_n$  consists of exactly K disconnected subgraphs that map on exactly to each manifold for some  $\eta \in (0, \delta)$ . Then for any  $\epsilon \in (0, 1)$ , there exists an N such that when n > N,  $A_n$  occurs with high probability.

#### 3.2 Intersecting Manifolds

In this section, we again consider the setting for the RDPG or GRDPG in which each community lies on a manifold in the latent space. However, this time, we do not assume that the manifolds are nonintersecting. We also restrict this case to one-dimensional manifolds which are each described by  $g_k : [0,1] \to \mathcal{X}$ . Then we define a mixture model as follows:

- 1. Draw  $t_1, ..., t_n \stackrel{\text{iid}}{\sim} F$  for probability distribution F with support [0, 1].
- 2. Draw  $z_1,...,z_n \stackrel{\text{iid}}{\sim} \text{Multinomial}(\alpha_1,...,\alpha_K)$ , the community labels.
- 3. Let each  $x_i = g_{z_i}(t_i)$  be the latent vector for vertex  $v_i$ , and collect the latent vectors into matrix  $X = \begin{bmatrix} x_1 & \cdots & x_n \end{bmatrix}^\top$ .
- 4. Draw  $A \sim \text{RDPG}(X)$  or  $A \sim \text{GRDPG}_{p,q}(X)$ .

**Theorem 2.** Let each  $g_k$  be smooth. Then K-curves clustering converges to a stationary point of the objective,  $\sum_k \sum_{i \in C_k} ||x_i - g_k(t_i)||^2$ .

*Proof.* K-curves clustering is a batch coordinate descent algorithm. Thus, in order to show that it converges to a stationary point, it is sufficient to show that each descent step decreases the objective function.

K-curves clustering assumes that the functional form of  $g_k$  is known. The choice of  $g_k$  affects the difficulty of the algorithm. As a balance between flexibility and ease of estimation, we consider the case where each  $g_k$  is a Bezier polynomial of degree R with coefficients  $p_k$ . Then we have  $g_k(t) = g(t; p_k) = \sum_{r=0}^R p_k^{(r)} \binom{R}{r} (1-t)^{R-r} t^r$ .

Given  $\{t_i\}$  and  $\{z_i\}$ , it is straightforward to obtain  $\hat{p}_k = \arg\min_{p} \sum_{k_i} ||x_{k_i} - g_k(t_{k_i}; p)||^2$ 

$$\hat{p}_k = (T_k^\top T_k)^{-1} T_k^\top X_k,$$

#### **Algorithm 2:** *K*-curves clustering.

**Data:** Adjacency matrix A, number of communities K, embedding dimensions p, q, stopping criterion  $\epsilon$ 

**Result:** Community assignments 1, ..., K, curves  $g_1, ..., g_K$ 

- 1 Compute X, the ASE of A using the p most positive and q most negative eigenvalues and their corresponding eigenvectors.
- 2 Initialize community labels  $z_1, ..., z_n$ .

```
з repeat
```

```
for k=1,...,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,...,K do

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

end

end
```

11 until the change in  $\sum_{k} \sum_{i \in C_k} ||x_i - g_k(t_i)||^2$  is less than  $\epsilon$ 

where  $T_k$  is an  $n_k \times (R+1)$  matrix with rows  $\left[ (1-t_{k_i})^R \quad (1-t_{k_i})^{R-1} t_{k_i} \quad \cdots \quad (1-t_{k_i}) t_{k_i}^{R-1} \quad t_{k_i}^R \right]$ . Estimation of  $\{t_i\}$  given  $\{z_i\}$  and  $\{p_k\}$  is more difficult. Each  $t_i$  can be estimated separately:

$$\hat{t}_i = \arg\min_t \|x_i - g(t; p_{z_i})\|^2.$$
(1)

This is equivalent to solving  $0 = (x_i - g(t; p_{z_i}))^{\top} (\dot{g}(t; p_{z_i}))$ . Setting  $c^{(s)} = \sum_{r=0}^{s} (-1)^{s-r} {R \choose r} p_{z_i}^{(r)}$  for  $s \neq 0$  and  $c^{(0)} = p_{z_i}^{(0)} - x_i$ , let  $c = \begin{bmatrix} c^{(0)} & \cdots & c^{(R)} \end{bmatrix}^{\top}$ . Then solving Eq. 1 is equivalent to finding the real roots of a polynomial with coefficients that are the sums of the reverse diagonals of  $CD^{\top}$ , where  $C_{ij} = c_{ij}(-1)^i {R \choose i}$  and  $D_{ij} = c_{i-1,j}(-1)^{i-1} {R-1 \choose i-1}$ .

**Theorem 3.** Let each  $g(\cdot; p_k)$  be a nonintersecting Bezier polynomial of order R, and a GRDPG is drawn from vectors that lie on the curves. Suppose we observe the true labels of  $m_k$  vertices from each community, and each  $m_k > R + 1$ . Suppose further that latent vectors  $x_j = g(t_i; p_{z_j})$  that correspond to vertices with observed labels are such that Then as  $n \to \infty$ , the proportion of misclustered vertices from K-curves clustering approaches 0 with probability 1.

#### **Algorithm 3:** Semi-supervised *K*-curves clustering.

**Data:** Adjacency matrix A, number of communities K, embedding dimensions p, q, stopping criterion  $\epsilon$ ,  $m_k \leq n_k$  known community assignments for each community

**Result:** Community assignments 1, ..., K, curves  $g_1, ..., g_K$ 

- 1 Compute X, the ASE of A using the p most positive and q most negative eigenvalues and their corresponding eigenvectors.
- 2 Fit curves  $g_1, ..., g_K$  using each of the  $m_1, ..., m_K$  points with known community labels by minimizing  $\sum_{j=1}^{m_i} \|x_j g_k(t_j)\|^2$ .
- **3** Assign labels  $z_1, ..., z_n$  to each  $x_1, ..., x_n$  by minimizing  $||x_i g_k(t_i)||^2$  for k, holding the initial known labels constant.

```
4 repeat
```

```
for k=1,...,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,...,K do

Assign z_i \leftarrow \arg\min_{\ell} \|x_i - g_{\ell}(t_i)\|^2, holding the known initial labels constant.

end
```

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

### 4 Examples

**Example 3.** Here, K = 2 with  $g_1(t) = \begin{bmatrix} t^2 & 2t(1-t) \end{bmatrix}^{\mathsf{T}}$  and  $g_2(t) = \begin{bmatrix} 2t(1-t) & (1-t)^2 \end{bmatrix}^{\mathsf{T}}$ . We draw  $n_1 = n_2 = 2^8$  points uniformly from each curve.

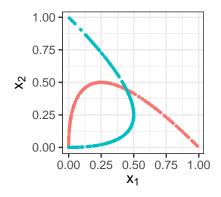


Figure 2: Latent positions, labeled by curve/community.

We draw  $A \sim \text{RDPG}(X)$  and obtain the following ASE:

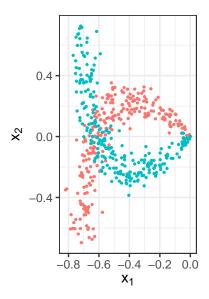


Figure 3: ASE of an RDPG drawn from the latent positions, labeled by curve/community.

We then try applying K-curves clustering to this graph. The first three are with random initial labels, forcing the intercept to be zero. The fourth initializes the labels randomly but allows the intercept to be nonzero. The fifth initializes the labels by spectral clustering with the normalized Laplacian, again forcing the intercept to be zero. The sixth also initializes via spectral clustering but allows the intercept to be nonzero.

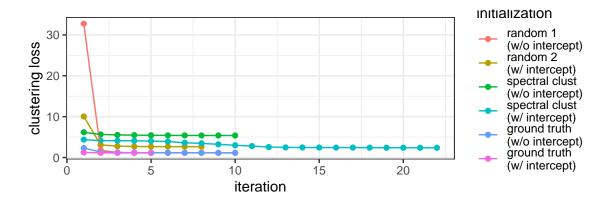


Figure 4: Clustering loss vs. iteration for each run of K-curve clustering.

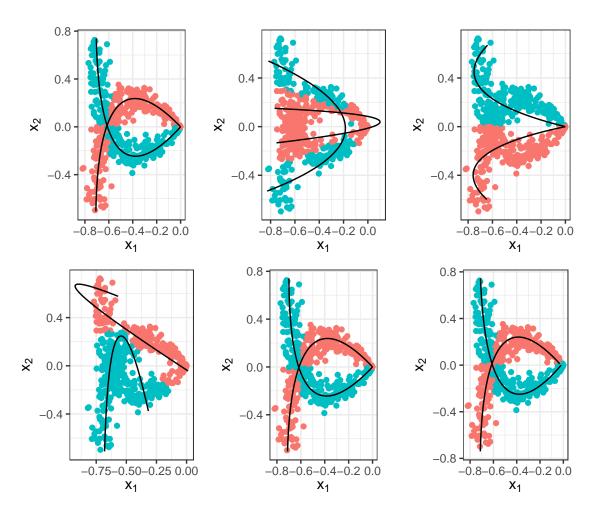
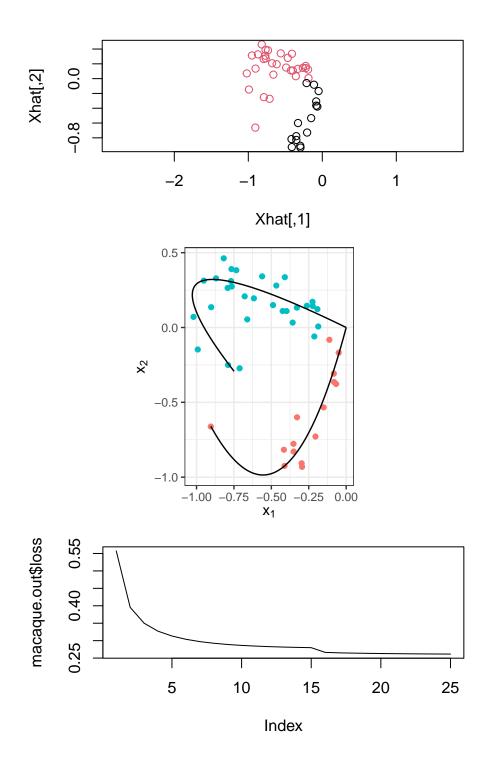
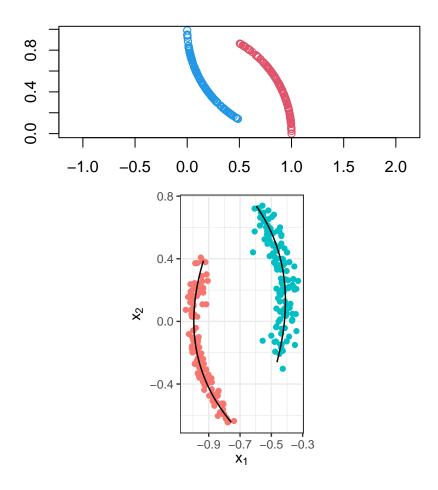


Figure 5: ASE labeled by estimated community labels for each initialization strategy.

Example 4 (Macaque visuotactile brain areas and connections (Négyessy et al. 2006)).



Example 5 (Non-intersecting curves).



# 5 Simulation Study

# 6 Discussion

### A Proofs of Theorems

In order to prove theorem 1, we first establish that the density of points within one manifold is sufficiently dense. The following lemma is based on lemma 2 of Trosset & Buyukbas (2020).

**Lemma 1.** Let  $x_1, ..., x_n \stackrel{\text{iid}}{\sim} F$  with support  $[0, 1]^r$ , and  $f(x) \geq a > 0$  everywhere on the support. Define  $H_n$  as the event that an  $\eta$ -neighborhood graph constructed from the sample is connected for any  $\eta > 0$ . Then for any  $\epsilon > 0$ , there exists  $N = O\left(\frac{\log \epsilon + r \log \eta - \frac{r}{2} \log r}{\log(1 - a\eta^r r^{-r/2})}\right)$  such that  $P(E_n) > 1 - \epsilon$  when  $n \geq N$ .

*Proof.* Divide the hypercube  $[0,1]^r$  into a grid of sub-hypercubes of side length at most  $\eta/\sqrt{r}$ .  $E_n$  is satisfied if each sub-hypercube contains at least one  $X_i$  from the sample.

$$P(H_n) = 1 - P(\text{some cells don't contain } X_i)$$

$$\geq 1 - \sum_{m=1}^{\lceil \sqrt{r}/\eta \rceil^r} \prod_{i=1}^{n} P(X_i \text{ is not in the } k^{th} \text{ hypercube})$$

$$\geq 1 - \lceil \sqrt{r}/\eta \rceil^r (1 - a\eta^r/r^{r/2})^n,$$

which approaches 1 as  $n \to \infty$ . Setting this quantity as  $\geq 1 - \epsilon$  and solving for n yields the desired rate.

**Lemma 2.** Let there be  $K \geq 2$  hypercubes  $C_1, ..., C_K$  of dimension  $r_1, ..., r_K$  in  $\mathbb{R}^d$  such that  $\delta = \min_{k \neq \ell} \min_{x_i \in C_k, x_j \in C_\ell} ||x_i - x_j|| > 0$ . Let  $F_k$  be a distribution with support  $C_k$  such that its density  $f_k$  is nonzero on the support. Let  $a = \min_k \min_t f_k(t) > 0$ . Define a mixture model as follows:

- 1. Draw labels  $z_1, ..., z_n \stackrel{\text{iid}}{\sim} \text{Multinomial}(\alpha_1, ..., \alpha_K)$ .
- 2. Draw latent vectors each as  $x_i \stackrel{\text{ind}}{\sim} F_{z_i}$ .

Define  $H'_n$  as the event that an  $\eta$ -neighborhood graph constructed from this sample consists of exactly K disconnected subgraphs for any  $\eta \in (0, \delta)$ . Then for any  $\epsilon \in (0, 1)$ , there exists an  $N = O\left(\frac{\log(1-(1-\epsilon)^{1/K})+d\log\eta-\frac{d}{2}\log d}{\alpha_{min}\log(1-a\eta^dd^{-d/2})}\right)$  such that when n > N,  $P(E_n) > 1 - \epsilon$ .

*Proof.* Let  $H^{(k)}$  be the event that lemma 1 holds for  $C_k$ . Then  $H^{(k)} = H_{n_k}$  where  $H_n$  is defined as in 1. Then  $P(H'_n) = P(H_{n_1})$  and ... and  $H_{n_k}$ .

$$P(H'_n) = \prod_k P(H_{n_k})$$

$$\geq \prod_k 1 - \lceil \sqrt{r_k} / \eta \rceil^{r_k} (1 - a \eta^{r_k} r_k^{-r_k/2})^{n_k}$$

$$\geq \prod_k 1 - \lceil \sqrt{d} / \eta \rceil^d (1 - a \eta^d d^{-d/2})^{\alpha_{\min} n}$$

$$\geq (1 - \lceil \sqrt{d} / \eta \rceil^d (1 - a \eta^d d^{-d/2})^{\alpha_{\min} n})^K,$$

which approaches 1 as  $n \to \infty$ . Setting this quantity to  $\geq 1 - \epsilon$  and solving for n yields the desired rate.

Proof of theorem 1.  $\Box$ 

# B Details on Fitting Bezier Curves with Noise

# References

Négyessy, L., Nepusz, T., Kocsis, L. & Bazsó, F. (2006), 'Prediction of the main cortical areas and connections involved in the tactile function of the visual cortex by network analysis', *European Journal of Neuroscience* **23**(7), 1919–1930.

**URL:** https://onlinelibrary.wiley.com/doi/abs/10.1111/j.1460-9568.2006.04678.x

Trosset, M. W. & Buyukbas, G. (2020), 'Rehabilitating isomap: Euclidean representation of geodesic structure'.

**URL:** https://arxiv.org/abs/2006.10858