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Latent structure blockmodels for **Bayesian spectral graph clustering**

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1. Latent position models and RDPGs

• Consider the adjacency matrix $\mathbf{A} = \{A_{ij}\} \in \{0,1\}^{n \times n}$ of a graph, where $A_{ij} = 1$ if node *i* connects to node *j*, and $A_{ij} = 0$ otherwise.



• Graph adjacency matrices can be modelled via latent **position models** (LPMs; Hoff et al., 2002):

2. Proposed methodology: latent structure blockmodels (LSBMs)

- Add a group structure to LSMs → latent structure blockmodels (LSBMs).
- Each node is assigned a latent membership $z_i \in \{1, \ldots, K\}$, with probabilities η_1, \ldots, η_K , with $\eta_k \ge 0$ and $\sum_{k=1}^K \eta_k = 1$.
- Each community is associated with a different one-dimensional structural support submanifold $\mathcal{S}_k \subset \mathbb{R}^d, \ k = 1, \dots, K$. Implicitly, $F = \sum_{k=1}^{K} \eta_k F_k$ is a mixture distribution with components F_1, \ldots, F_K supported on $\mathcal{S}_1, \ldots, \mathcal{S}_K$.
- Assuming community allocations $z = (z_1, \ldots, z_n)$, the latent positions are obtained as

 $\boldsymbol{x}_i | z_i \sim F_{z_i}, \ i = 1, \dots, n,$

where F_{z_i} is the distribution of the community-specific transformation $f_{z_i}(\theta)$ of a shared univariate random variable $\theta \sim G$. • G is common to all the nodes, and the pair (θ_i, z_i) , where $\theta_i \sim G$, determines the latent position x_i through f_{z_i} , such that:

 $\boldsymbol{x}_i = \boldsymbol{f}_{z_i}(heta_i).$

3. A Bayesian model for LSBMs

4. Posterior inference

$\boldsymbol{x}_i \stackrel{iid}{\sim} F \rightarrow \mathbb{P}(A_{ij} = 1 | \boldsymbol{x}_i, \boldsymbol{x}_j) = \kappa(\boldsymbol{x}_i, \boldsymbol{x}_j) \rightarrow$

- LPMs are built on a powerful idea: expressing edgespecific probabilities through latent node features $x_i \in \mathcal{X} \subseteq \mathbb{R}^d$, using a kernel function $\kappa : \mathcal{X} \times \mathcal{X} \to [0, 1]$. If the inner product is used, the model is known as ran-
- **dom dot product graph** (RDPG; Athreya et al., 2018):

 $A_{ij}|\boldsymbol{x}_1,\ldots,\boldsymbol{x}_n \sim \mathsf{Bernoulli}(\boldsymbol{x}_i^{\mathsf{T}}\boldsymbol{x}_j).$

• RDPGs include many popular network models:

- Stochastic blockmodels (SBMs): $x_i = \mu_{z_i}$ for a community $z_i \in \{1, \ldots, K\}$, giving a betweencommunity connection probability $B_{k\ell} = \boldsymbol{\mu}_k^{\mathsf{T}} \boldsymbol{\mu}_\ell$;
- Degree-corrected SBMs: $m{x}_i =
 ho_i m{\mu}_{z_i}$ for $z_i \in$ $\{1, \ldots, K\}$ and degree-correction $\rho_i \in (0, 1)$.
- In RPDGs, the latent positions are **estimated via spectral decomposition** of the adjacency matrix.

Definition 1: Adjacency spectral embedding (ASE)

For an integer $d \in \{1, \ldots, n\}$ and a binary symmetric adjacency matrix $\mathbf{A} \in \{0, 1\}^{n \times n}$, the *d*-dimensional adjacency spectral embedding $\mathbf{X} = [\hat{\boldsymbol{x}}_1, \dots, \hat{\boldsymbol{x}}_n]^{\mathsf{T}}$ of \mathbf{A} is $\hat{\mathbf{X}} = \mathbf{\Gamma} \mathbf{\Lambda}^{1/2} \in \mathbb{R}^{n imes d},$

where Λ is a $d \times d$ diagonal matrix containing the absolute

 $\hat{\boldsymbol{x}}_i | \theta_i, \boldsymbol{f}_{z_i}, \boldsymbol{\sigma}_{z_i}^2 \sim \mathbb{N}_d \left\{ \boldsymbol{f}_{z_i}(\theta_i), \boldsymbol{\sigma}_{z_i}^2 \mathbf{I}_d \right\}, \ i = 1, \dots, n,$ $\theta_i \sim \mathbb{N}(\mu_{\theta}, \sigma_{\theta}^2), \ i = 1, \dots, n,$ $f_{k,j} | \sigma_{k,j}^2 \sim \mathsf{GP}(0, \sigma_{k,j}^2 \xi_{k,j}), \ k = 1, \dots, K, \ j = 1, \dots, d,$ $\sigma_{k,j}^2 \sim \mathsf{IG}(a_0, b_0), \ k = 1, \dots, K, \ j = 1, \dots, d,$ $z_i | \boldsymbol{\eta}, K \sim \mathsf{Categorical}(\boldsymbol{\eta}), \ i = 1, \dots, n,$ $\eta | K \sim \mathsf{Dirichlet}(\nu/K, \ldots, \nu/K),$ $K \sim \text{Geometric}(\omega),$

where $a_0, b_0, \nu, \omega, \sigma_{\theta}^2 \in \mathbb{R}_+, \mu_{\theta} \in \mathbb{R}$, and $\xi_{k,j}$ is a positive semi-definite kernel function.

- After marginalisation of $(f_{k,j}, \sigma_{k,j}^2)$ and η , inference is limited to the community allocations z and parameters θ .
- The posterior distribution $p(\boldsymbol{z}, \boldsymbol{\theta}, K \mid \mathbf{X})$ is analytically intractable; inference is performed using MCMC methods.
 - Resample the community allocations z;
 - Resample the latent parameters θ ;
 - Split-merge communities;
 - Add or remove an empty community;
 - If prior on kernels is used: resample kernels.

• The kernel function is usually assumed to be in inner product form, with Zellner's *g*-prior on the scaling matrix.

5. Examples of LSBMs: SBMs, DCSBMs and quadratic LSBMs

• Kernels – SBM: $\xi_{k,j}(\theta, \theta') = \Delta_{k,j}, \ \Delta_{k,j} \in \mathbb{R}_+$; DCSBM: $\xi_{k,j}(\theta, \theta') = \theta \theta' \Delta_{k,j}$; Quadratic: $\xi_{k,j}(\theta, \theta') = (\theta, \theta^2) \Delta_{k,j}(\theta', \theta'^2)^\intercal$.

(a): *SBM:* $f_{k,j}(\theta_i) = \nu_{k,j}$









values of the d largest eigenvalues in magnitude, and Γ is a $n \times d$ matrix containing corresponding eigenvectors.

- For directed graphs, the singular value decomposition (SVD) is used.
- In practice, spectral embeddings often exhibit manifold structure (Rubin-Delanchy, 2020).
- Spectral graph clustering consists in unsupervised detection of groups of nodes from spectral embeddings.



 There are two simultaneous challenges in graph clustering via spectral embedding under the RDPG:

Manifold structure **Group** structure

Group-specific manifolds.

Manifold structure is accounted for by latent structure



Figure 1: Scatterplots of the two-dimensional ASE of simulated graphs arising from simple models, and true underlying latent curves (in black). For each graph, n = 1000 with K = 2 communities of equal size. For (a) and (b), $\nu_1 = [3/4, 1/4]$, $\nu_2 = [1/4, 3/4]$ and $\theta_i \sim Beta(1,1)$. For (c), $\alpha_k = [-1, -4]$, $\beta_k = [1,1]$, $\gamma_k = [0,0]$ and $\theta_i \sim Beta(2,1)$.

Method	$ LSBM(\hat{\mathbf{X}})$	$\text{GMM}(\hat{\mathbf{X}})$	$\text{GMM}(\tilde{\mathbf{X}})$	$SCSC(\hat{\mathbf{X}})$	$PGP(\hat{\mathbf{X}})$	HLouvain	$HClust(\hat{\mathbf{X}})$
SBM	1.0	1.0	1.0	1.0	1.0	1.0	1.0
DCSBM	0.853	0.802	0.838	0.887	0.842	0.827	0.411
Quadratic LSBM	0.838	0.620	0.712	0.636	0.691	0.582	0.101

Table 1: ARI for communities estimated using LSBM and alternative methodologies on the embeddings in Figure 1.

6. Results on three networks



0.4



(c): ICL computer laboratories network



models (LSM, Athreya et al., 2021):

- The latent positions $x_i \stackrel{iid}{\sim} F$ are determined by draws from an underlying univariate distribution G on [0, 1], inducing F on a univariate submanifold $\mathcal{S} \subset \mathbb{R}^d$.
- The distribution F on S is the distribution of the transformation $f(\theta)$ of a univariate random variable $\theta \sim G$, where $f: [0,1] \to S$ is a function mapping θ to S.
- In simple terms, each node is assigned a draw θ_i from the underlying distribution G, representing how far along \mathcal{S} the corresponding latent position lies:

 $\boldsymbol{x}_i = \boldsymbol{f}(\theta_i).$

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Figure 2: Two-dimensional embeddings, estimated communities and true labels for three real-world dataset.

Method	$ LSBM(\hat{\mathbf{X}})$	$\text{GMM}(\hat{\mathbf{X}})$	$\text{GMM}(\tilde{\mathbf{X}})$	$\text{SCSC}(\hat{\mathbf{X}})$	$PGP(\hat{\mathbf{X}})$	HLouvain	$\text{HClust}(\hat{\mathbf{X}})$
Drosophila connectome	0.875	0.599	0.585	0.667	0.555	0.087	0.321
ICL computer laboratories	0.940	0.659	0.766	0.921	0.895	0.602	0.139

Table 2: ARI for communities estimated using LSBM and alternative methodologies on the Drosophila and ICL laboratories networks.

References

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1.0

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Paper and python library lsbm

Paper

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