Stochastic Block Model Prior with Ordering Constraints for Gaussian Graphical Models

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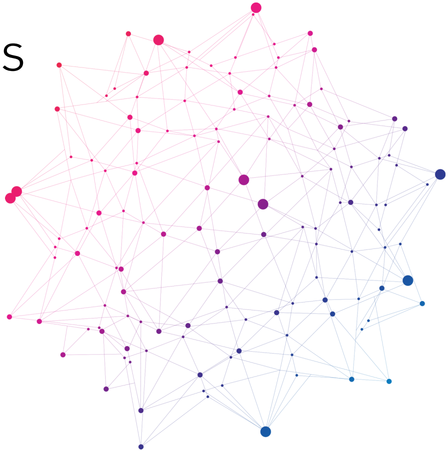

Bayesian Statistics
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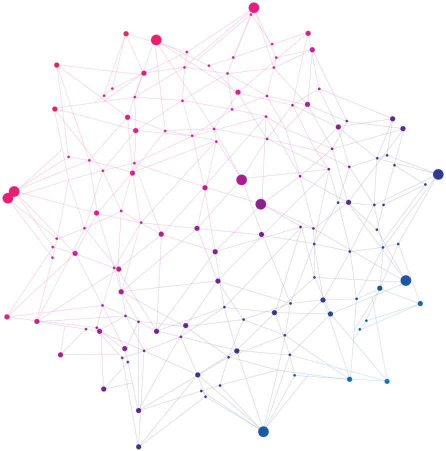

BACKGROUND

GAUSSIAN GRAPHICAL MODELS

Models for the **conditional dependence structure** among variables, represented through an undirected graph $G = (V, E)$

$$\boldsymbol{y}_1, \dots, \boldsymbol{y}_n \mid \boldsymbol{K} \overset{\text{iid}}{\sim} \mathcal{N}_p(\boldsymbol{0}, \boldsymbol{K}^{-1})$$

Conditional independence described through a **map** between a **graph** and a family of multivariate **probability models**

$$Y_i \perp\!\!\!\perp Y_j \mid Y_{-(ij)} \iff (i,j) \notin E \iff k_{ij} = 0$$

Usual prior for $\boldsymbol{K}$ conditionally to the graph is a G-Wishart

$$\boldsymbol{K} \mid G \sim \text{G-Wishart}(b, D)$$

G is a r.v. in the space of undirected graphs with p nodes.
If we assume a possible **grouping** of the variables, we need a prior $\pi(G)$ that induces a **block structure on its adjacency matrix**.

STOCHASTIC BLOCK MODELS FOR THE PRIOR ON G

Given a random network, SBM **infer a node partition** based on similarity of connectivity patterns. Let

- H be the fixed number of clusters
- $\boldsymbol{z} \in \mathbb{R}^p$ be the vector of group memberships, $z_i \in \{1, \ldots, H\}$

Then the model of the graph conditionally on $\boldsymbol{z}$ is the following

$$
\begin{aligned}
P((i,j) \in E \mid \boldsymbol{z}, Q) &= Q_{z_i z_j}, \text{ independent} \\
Q_{rs} &\overset{\text{ind}}{\sim} \mathrm{Beta}(a, b), \quad 1 \leq r \leq s \leq H \\
\boldsymbol{z} &\sim f_z(\boldsymbol{z})
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Problems:

- How to **identify the number of clusters** H?
- How to model **constraints on the ordering of the nodes** when generating the partition?

CHANGEPOINT MODELS

Let $\boldsymbol{y} = (y_1, \dots, y_n)$ be **ordered** observations, each depending on a parameter ϑ_i. Consider a process where the underlying generating mechanism changes at time τ_j, $j = 1, \dots, k+1$, where τ_j, k are unknown. The likelihood can be modeled as

$$f(y_1, \dots, y_n \mid \vartheta_1, \vartheta_2, \dots, \vartheta_{k+1}, \boldsymbol{z}) = \prod_{j=1}^{k+1} \prod_{i=\tau_{j-1}+1}^{\tau_j} f(y_i \mid \vartheta_j), \qquad k = \sum_{i=1}^{n-1} z_i$$

where τ_j are called **changepoints** and $z_i = 1$ if i is a changepoint, 0 otherwise. We are interested in **generating a random partition with ordering constraints**

$$\pi(\boldsymbol{z}, \boldsymbol{\vartheta} \mid \boldsymbol{y}) \propto f(\boldsymbol{y} \mid \boldsymbol{\vartheta}, \boldsymbol{z}) \pi(\boldsymbol{\vartheta} \mid \boldsymbol{z}) \pi(\boldsymbol{z})$$

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Martínez and Mena 2014 assign

$$P\left(\rho_p = \{C_1, \ldots, C_M\}\right) = p'(n_1, \ldots, n_k) = \begin{cases} \binom{n}{n_1, \ldots, n_k} \frac{1}{k!} p(n_1, \ldots, n_k), & \rho_p \text{ admissible} \\ 0, & \rho_p \text{ not admissible} \end{cases}$$

where $n_j = |C_j|$, $p(n_1, \ldots, n_k)$ any Exchangeable Partition Probability Function (EPPF).

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The vector $\boldsymbol{z}$ is derived by setting

$$z_i = m \iff i \in C_m, \quad i = 1, \ldots, p, \quad m = 1, \ldots, M.$$

PROJECT GOALS AND NEXT STEPS

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Goal: propose a **new prior** that accounts for

- Ordering Constraint: taking advantage of the study of changepoint models
- Block Structure: using a stochastic block model prior

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\boldsymbol{y}_1, \dots, \boldsymbol{y}_n \mid \boldsymbol{K} &\overset{\text{iid}}{\sim} \mathcal{N}_p(\mathbf{0}, \boldsymbol{K}^{-1}) \\
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P((i,j) \in E \mid \boldsymbol{z}, Q) &= Q_{z_i z_j}, \text{ independent} \\
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Next steps:

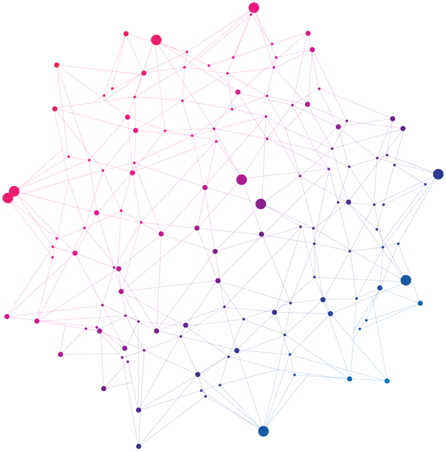
- understand the nonparametric prior on ordered partitions
- implement the sampling strategy

MAIN REFERENCES

- Benson, A. and N. Friel (2018). “Adaptive MCMC for Multiple Changepoint Analysis with Applications to Large Datasets”. In: Electronic Journal of Statistics 12.2.
- Colombi, A., R. Argiento, L. Paci and A. Pini (2022). “Learning block structured graphs in Gaussian graphical models”. In: arXiv preprint arXiv:2206.14274.
- Legramanti, S., T. Rigon, D. Durante and D. B. Dunson (2022). “Extended stochastic block models with application to criminal networks”. In: The Annals of Applied Statistics 16.4, pp. 2369–2395.
- Martínez, A. F. and R. H. Mena (2014). “On a Nonparametric Change Point Detection Model in Markovian Regimes”. In: Bayesian Analysis 9.4.
- Mohammadi, A. and E. C. Wit (2015). “Bayesian Structure Learning in Sparse Gaussian Graphical Models”. In: Bayesian Analysis 10.1.

Thank you!

Any questions?



STOCHASTIC BLOCK MODELS FOR THE PRIOR ON G

$$G_{ij} \mid \Theta, \boldsymbol{z} \overset{\text{iid}}{\sim} \text{Be}(\vartheta_{ij}),\ G \in \mathbb{R}^{p\times p}, \quad \vartheta_{ij} = \Theta_{z_i z_j}, \quad 1 \le i < j \le p$$
$$\Theta_{z_i z_j} \overset{\text{iid}}{\sim} \text{Beta}(\alpha, \beta)$$
$$\boldsymbol{z} \overset{\text{iid}}{\sim} \pi_z(\boldsymbol{z}), \quad \boldsymbol{z} \in \mathbb{R}^p$$

Θ can be marginalized out via beta-binomial conjugacy.

From Colombi et al. 2022

CHOOSING THE NUMBER OF CLUSTERS H

H is usually chosen using data driven methods **before** estimating the model. However

- uncertainty quantification for H at this stage is ignored
- the model does not account for new clusters (**prediction**)

Among others, Legramanti et al. 2022 proposed the **Extended Stochastic Block Models (ESBM)**, which use priors for $\boldsymbol{z}$ that naturally allow to adaptively modify the number of groups H, e.g.,

- Finite Dirichlet
- Infinite Dirichlet
- Finite mixtures with a random number of components

None of the ESBM models pose constraints on the ordering of the nodes when generating the partition, that may be of relevance in a real-life context (e.g., gene expression).