

Clustering species with residual covariance matrix in Joint Species Distribution models

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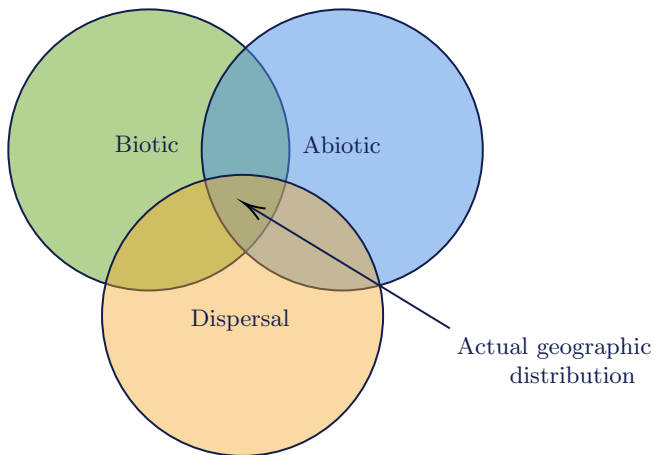
Applications du Bayesian Unified Group of Statisticians
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Species distribution



The three factors that determine the actual distribution of a species [Soberon and Peterson, 2005].

Species distribution models (SDMs)

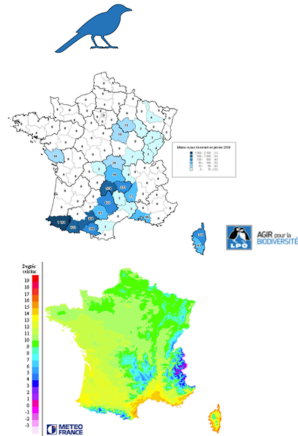
Species

Species Distribution
Data

Environmental
covariates
(characteristics)

$\{y\}_{i=1}^n$

$\{x\}_{i=1}^n$



Species distribution models (SDMs)

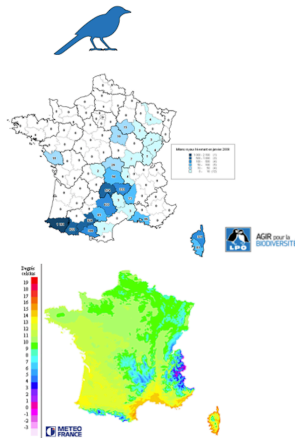
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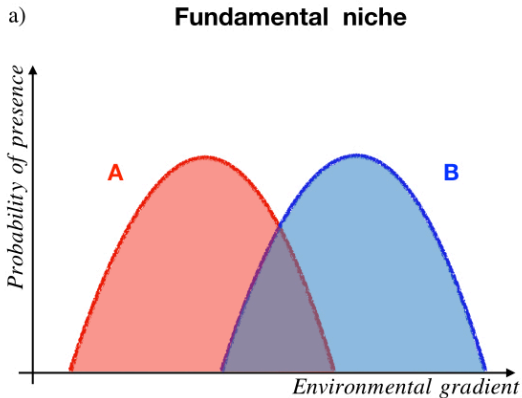
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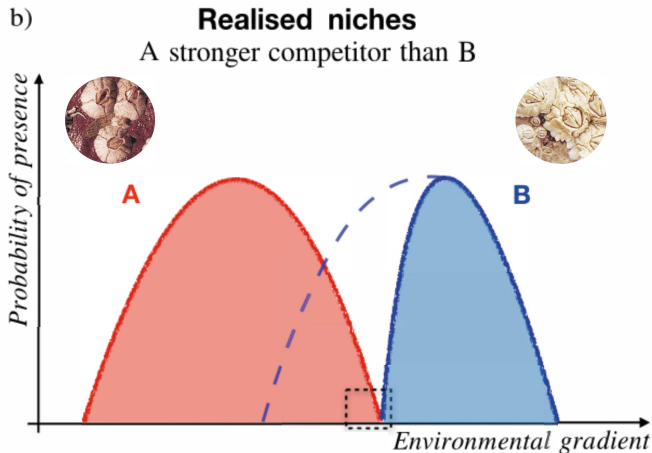
$$P(y_i = 1) = \Phi(\beta^T x_i)$$

Species distribution models: fundamental niche



[Poggiato et al., 2021]

Species distribution models: realized niche



[Poggiato et al., 2021]

Species distribution models

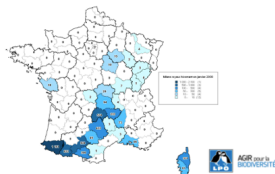
Species

$$j = \{1, \dots, S\}$$



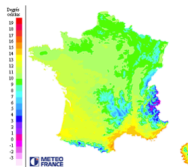
Species Distribution
Data

$$\{y_{ij}\}_{i=1}^n$$



Environmental
covariates
(characteristics)

$$\{x\}_{i=1}^n$$



Joint species distribution models (JSDMs)

Formally: Consider $j = 1, \dots, S$ species, $i = 1, \dots, n$ sites and $\mathbf{x}_i = \{x_{ik}\}_{k=1}^K$ K environmental covariates. **Response variable** $y_{ij} \in \{0, 1\}^S$ is modelled as follows:

$$y_{ij} = \mathbb{I}(z_{ij} > 0)$$

$$\mathbf{z}_i = \boldsymbol{\beta} \mathbf{x}_i + \mathbf{e}_i$$

$$\mathbf{e}_i \stackrel{\text{iid}}{\sim} N_S(0, \mathbf{R}),$$

- $\boldsymbol{\beta} \in \mathbb{R}^{K \times S}$, $\boldsymbol{\beta}_j$ represent species-specific response to the environment.
- \mathbf{R} correlation matrix: reflects species co-occurrence pattern not explained by selected abiotic covariates.

Existing approaches: Pollock et al. [2014], Clark et al. [2017] Ovaskainen et al. [2017], Harris [2015], Vanhatalo et al. [2020].

Problems:

- inter-species dependencies captured by $\mathbf{R} \neq$ species interactions.

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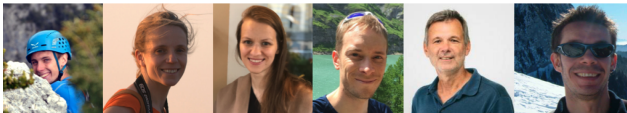
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Problems:

- inter-species dependencies captured by $\mathbf{R} \neq$ species interactions.
- computationally heavy as models have $O(S^2)$ parameters



On the interpretations of Joint Species Distribution Models

Giovanni Poggiato, Tamara Münkemüller, Daria Bystrova, Julyan Arbel, James S. Clark and Wilfried Thuiller. *Trends Ecol. Evol.* 2021

Questions

- Can JSDMs improve the estimation of species fundamental niches?
- What can the residual correlation matrix tell us about biotic interactions?
- When and why do JDSMs outperform SDMs?



Clustering species with residual covariance matrix in Joint Species Distribution models.

Daria Bystrova, Giovanni Poggiato, Billur Bektas, Julyan Arbel, James S. Clark, Alessandra Guglielmi and Wilfried Thuiller. *Front. Ecol. Evol.* 2021

Questions

1. Can prior knowledge, combined with dimension reduction on the structure of the residual covariance matrix, improve model inference in JSDM?
2. Can estimated clusters be interpreted in ways that help us understand species communities?

Motivation

- models have $O(S^2)$ parameters \implies dimension reduction approaches.
- large number of parameters in $\mathbf{R} \implies$ difficulties in interpretation
- use prior knowledge in JSDMs

Existing approaches:

- Latent variable models(LVM) [Warton et al., 2015], GJAM [Taylor-Rodriguez et al., 2017], HMSC [Ovaskainen et al., 2016], BORAL [Hui, 2016];
- efficient parallel sampling Chen et al. [2018], sjSDM [Pichler and Hartig, 2020]

Our proposal: a novel framework that allows for a clustering of residual associations that makes use of prior information.

Latent variable models

Formally : Consider $j = 1, \dots, S$ species, $i = 1, \dots, n$ sites and $\mathbf{x}_i = \{x_{ik}\}_{k=1}^K$ K environmental covariates, $y_{ij} \in \{0, 1\}^S$ is modelled as follows:

$$y_{ij} = \mathbb{I}(z_{ij} > 0),$$
$$\mathbf{z}_i = \beta \mathbf{x}_i + \mathbf{\Lambda} \boldsymbol{\omega}_i + e_i, \quad e_i \stackrel{\text{iid}}{\sim} N_S(0_S, \sigma_\epsilon^2 \mathbf{I}_S), \quad \omega_{ij} \stackrel{\text{iid}}{\sim} N(0, 1).$$

- $S \times r$ matrix $\mathbf{\Lambda}$ is the **factor loading** matrix
- r -dimensional Gaussian random vectors $\boldsymbol{\omega}_i$ are called **latent factors**
- $r \ll S$: approximating $\boldsymbol{\Sigma}$ with $\tilde{\boldsymbol{\Sigma}} = \mathbf{\Lambda} \mathbf{\Lambda}^T + \sigma_\epsilon^2 \mathbf{I}_S$.

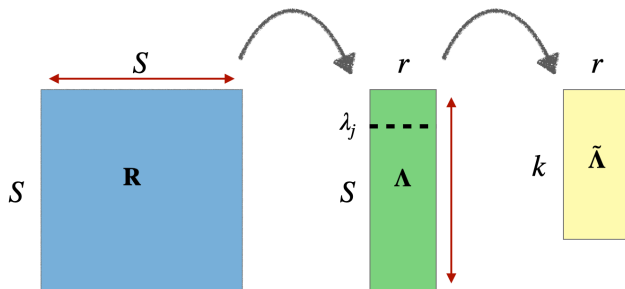
Further dimension reduction [Taylor-Rodriguez et al., 2017]:

Reducing $\mathbf{\Lambda}$ to $\tilde{\mathbf{\Lambda}}$ by clustering rows of $\mathbf{\Lambda}$

Clusters: species that share the same rows of $\mathbf{\Lambda}$ = species that **share the same residual correlation with respect to other species**.

→ cluster species depending on their associations with respect to other species.

Further dimension reduction



Clustering the rows $\lambda_j, j = 1, \dots, S$ in Λ with Dirichlet process (**DP**):

$$\begin{aligned}\lambda_j &| G \stackrel{\text{iid}}{\sim} G, \quad j = 1, \dots, S, \\ G &\sim \text{DP}(\alpha H),\end{aligned}$$

Dirichlet process

Definition(Dirichlet process)[Ferguson, 1973]

Let H be a distribution over Θ and $\alpha > 0$. We say that G is a Dirichlet Process, namely $G \sim DP(\alpha H)$ if for any finite measurable partition $\{A_1, \dots, A_r\}$ of Θ , we have:

$$(G(A_1), \dots, G(A_r)) \sim Dir(\alpha H(A_1), \dots, \alpha H(A_r)),$$

where H is called base distribution, and α the concentration parameter. The Dirichlet process (DP) is a central Bayesian nonparametric (BNP) prior.

The DP has almost surely discrete realisations[Sethuraman, 1994]:

$$G = \sum_{k=1}^{\infty} \pi_k \delta_{\theta_k},$$

where $\theta_k \sim H$

if $X_1, \dots, X_n \mid G \stackrel{\text{iid}}{\sim} G \quad i = 1, \dots, n \implies (X_1, \dots, X_n)$ feature K_n distinct observations $(X_1^*, \dots, X_{K_n}^*)$ with frequencies n_1, \dots, n_k such that $\sum_{i=1}^{K_n} n_i = n$.

Contribution

Clustering with BNP priors

- advantage of the BNP prior: no need to specify the exact number of clusters.
- BNP prior induce prior on the number of clusters K_n .
- In case of the DP process:
 - we can fix the features of the prior distribution on K_n using α
 - concentration parameter α has a strong effect on the posterior distribution of the number of clusters De Blasi et al. [2015].

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Contribution:

1. We propose to incorporating prior knowledge on the number of species that share residual associations that improves clustering properties.
2. We introduce Pitman–Yor process, a more flexible Bayesian nonparametric prior, which is less sensitive to miscalibration than the Dirichlet process.

Contribution

First approach (DP_c):

We consider prior distribution for the precision parameter α :

$$\alpha \sim \text{Ga}(\nu_1, \nu_2)$$

→ use Dirichlet multinomial process [Muliere and Secchi, 2003] for approximation of DP

→ calibrate prior on K_n by calibrating prior on α : $\mathbb{E}[K_S] = K^*$, where K^* prior knowledge on the number of clusters

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→ calibrate prior on K_n by calibrating prior on α : $\mathbb{E}[K_S] = K^*$, where K^* prior knowledge on the number of clusters

Second approach (PY_c):

Use more flexible Pitman–Yor process (PY):

$$\begin{aligned}\lambda_j &| G \stackrel{\text{iid}}{\sim} G, \quad j = 1, \dots, S, \\ G &\sim \text{PY}(\alpha, \sigma, H),\end{aligned}$$

where H is the base measure, α is the concentration parameter, and σ is the discount parameter.

→ use Pitman–Yor multinomial process [Lijoi et al., 2020] for approximation of PY

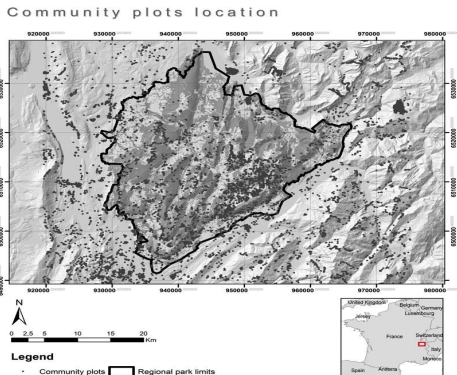
→ calibrate prior on K_n , by calibrating parameters α, σ : $\mathbb{E}[K_S] = K^*$ and $\mathbb{V}[K_S]$ to reflect the desired level of uncertainty.

Specification of concentration parameter α

Model	Concentration parameter α	Reference
DP	Fixed (number of species)	Taylor-Rodriguez et al. [2017]
DP_c	$\text{Ga}(\nu_1, \nu_2)$ s.t $\mathbb{E}[K_S] = K^*$	Ours
PY_c	Fixed, s.t $\mathbb{E}[K_S] = K^*$	Ours + Lijoi et al. [2020]

K^* is the prior ecological belief on the number of groups of species with the same residual correlation structure.

Case study: The Bauges National Regional Park



The dataset contains the presences and absences of 111 plant species in 1139 sites. Thuiller et al. [2018]

- Prior knowledge on number of groups in the species interaction network: 16 Plant Functional Groups (PFGs). ($\mathbb{E}[K_S] = 16$)
- We splitted the sites into training and test set, and took covariates as in Thuiller et al. [2018].

Ecological representation of the clusters

Traits:

Landolt nutrient indicator, Landolt lightindicator, height (in the logarithmic scale), specific leaf area (SLA), leaf dry matter content (LDMC), leaf carbon concentration (LCC), and leaf nitrogen concentration (LNC).

Grouping traits with a similar role in the community assembly process:

- competitive effect (height, SLA, LDMC, LCC, LNC)
- tolerance to abiotic and biotic conditions (Landolt nutrient indicator, Landolt lightindicator)
- interaction via light resources (height, SLA, Landolt light indicator)
- interaction via soil resources (LNC, Landolt nutrient indicator).

$$\text{Species grouped-trait ratio} = \frac{\text{mean}(\text{distance to other species})_{\text{within cluster}}}{\text{mean}(\text{distance to other species})_{\text{all species}}}$$

Clustering analysis

posterior expected number of clusters:

describes the distribution of the number of clusters in Markov chain Monte Carlo (MCMC) samples.

Summarize the **posterior distribution of the clusters** for **DP**, **DP_c** and **PY_c**.

Optimal cluster estimate from Wade and Ghahramani [2018]:

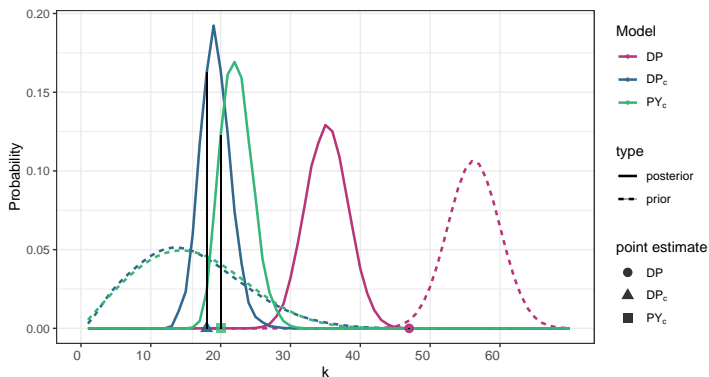
$$c^* = \arg \min_{\hat{c}} \mathbb{E}[L(c, \hat{c}) \mid \mathbf{Y}_{1:n}] = \arg \min_{\hat{c}} \sum_c L(c, \hat{c}) p(c \mid \mathbf{Y}_{1:n}), \quad (1)$$

where $p(c \mid \mathbf{Y}_{1:n})$ is posterior distribution of partition c .

the number of clusters of the estimated clustering:

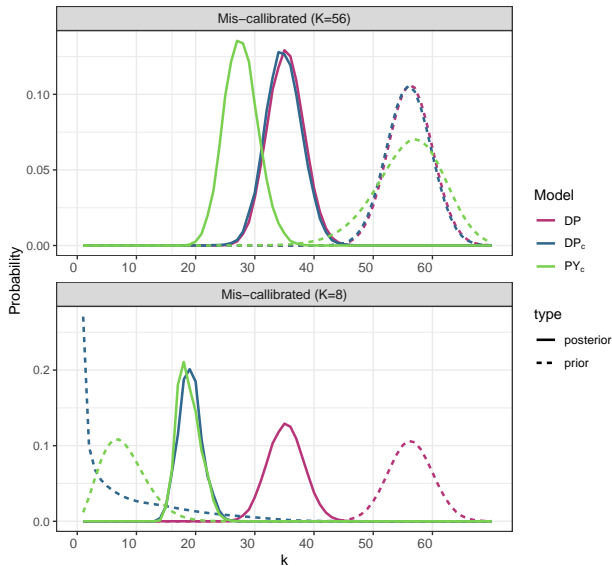
represents the number of clusters in the single partition that best represents the posterior distribution of the clusters in the MCMC samples

Results: posterior number of clusters



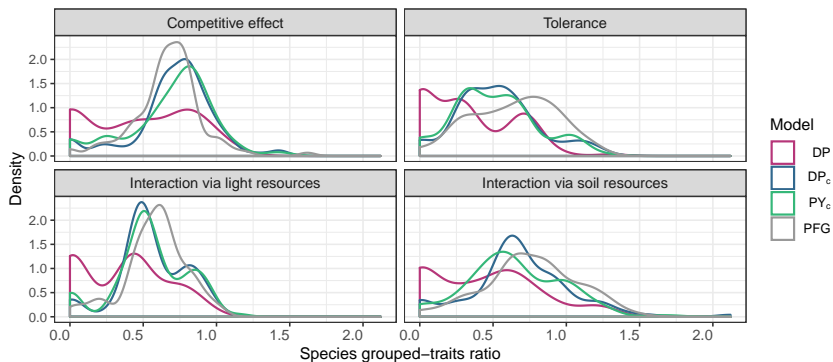
Prior distribution and posterior estimation of the number of clusters corresponding to **DP**, **DP_c** , **PY_c** models.

Results: sensitivity



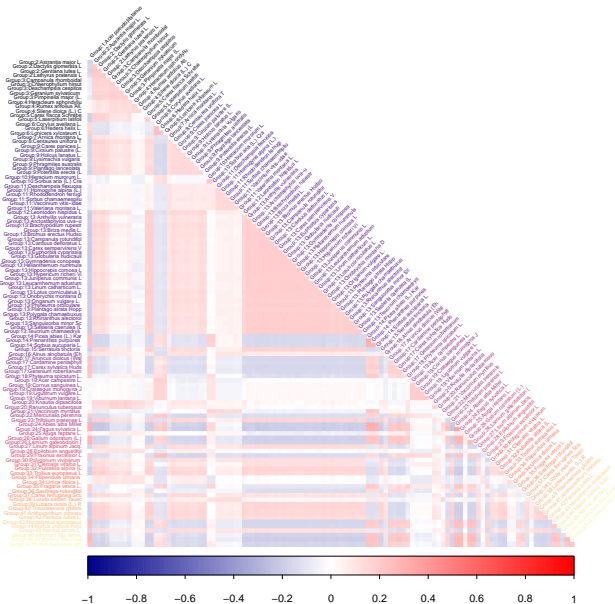
Prior and posterior distribution of the number of clusters for the models DP_c , PY_c .

Results: clusters interpretation

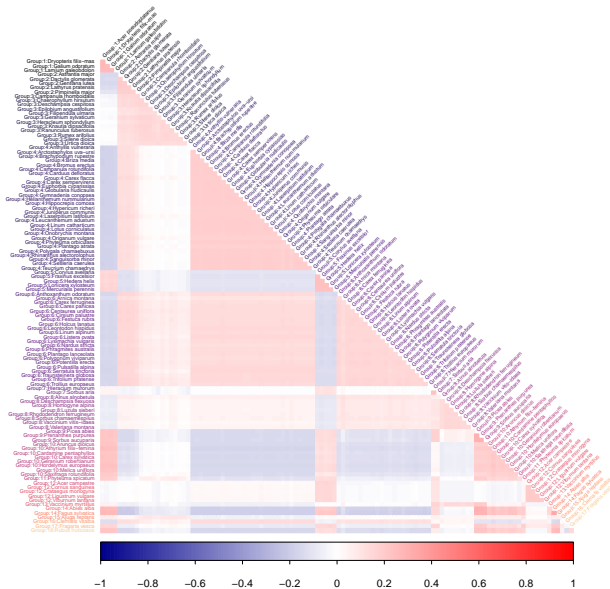


Distribution of species grouped-trait ratio. (DP, DP_c, PY_c)

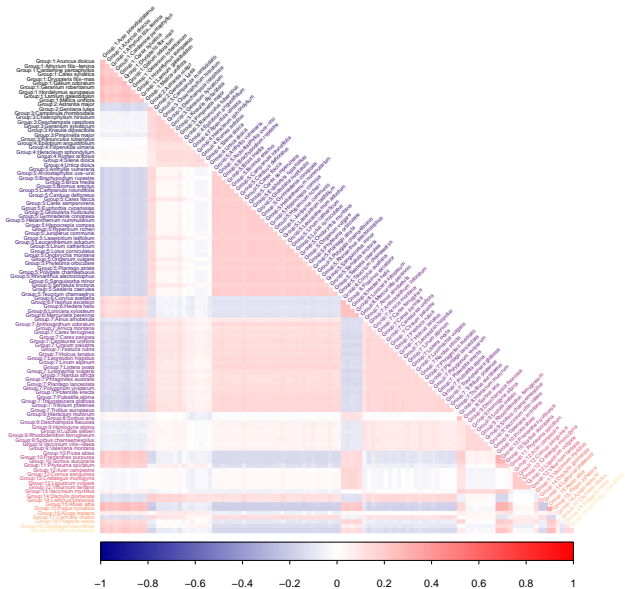
Results: residual covariance matrix DP



Results: residual covariance matrix DP_c



Results: residual covariance matrix PY_c



Conclusion

- (i) Our proposed statistical framework allows an additional but ecologically meaningful dimension reduction of JSDMs and includes prior knowledge in the residual covariance matrix.
- (ii) The case study shows that the obtained clusters of species are ecologically meaningful, and correlated with functional traits.

Further directions

- we focus on estimation precision matrix with block-diagonal structure.

Links

- Paper: <https://www.frontiersin.org/articles/10.3389/fevo.2021.601384>
- Code: https://github.com/dbystrova/GJAM_clust

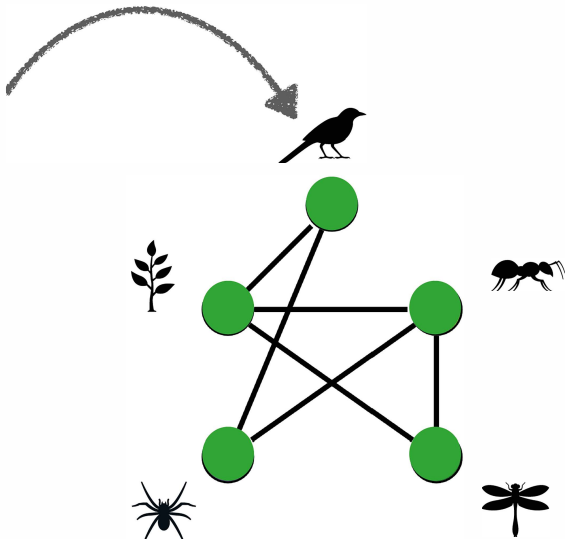
Further directions

Bayesian block-diagonal graphical models via the Fiedler prior
Joint work with **Julyan Arbel** and **Mario Beraha**

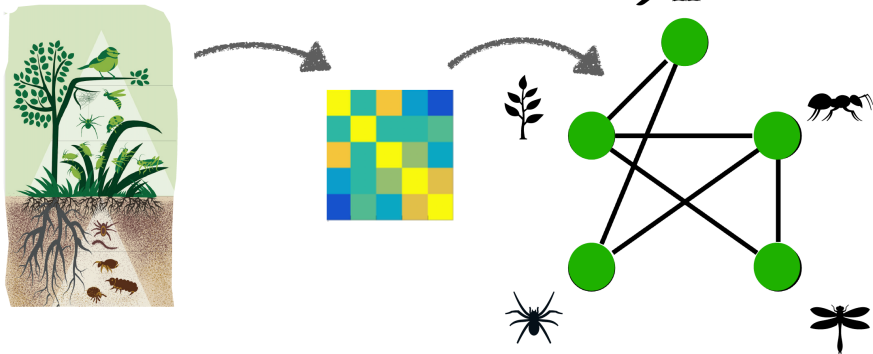
Structure learning



Thakur [2020]



Structure learning



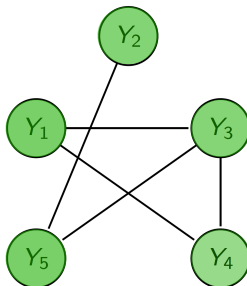
Gaussian graphical models

- associate p species with the components of a p -variate random vector $\mathbf{Y} = (Y_1, \dots, Y_p) \sim N_p(0, \Sigma)$
- n realizations of the vector \mathbf{Y}
- precision matrix $\Theta = \Sigma^{-1}$ is associated to partial correlation matrix.

Precision matrix

A zero at element ij of **the precision matrix Θ** corresponds to conditional independence of Y_i and Y_j given the other variables Y_{-ij}

$$\Theta = \begin{pmatrix} * & 0 & * & * & 0 \\ 0 & * & 0 & 0 & * \\ * & 0 & * & * & * \\ * & 0 & * & * & 0 \\ 0 & * & * & 0 & * \end{pmatrix}$$



Contribution

Inferential goals: estimation of the precision matrix Θ .

Problem

- Small sample setting: the number p of variables is greater than the number n of samples

Solutions:

- Graphical Lasso [Friedman et al., 2008], **Cluster Graphical Lasso** [Tan et al., 2015],
- Bayesian: Bayesian Graphical Lasso [Wang, 2012], Graphical Horseshoe [Li et al., 2019], G-Wishart prior [Mohammadi and Wit, 2015].

Our proposal:

- **Fiedler prior** shrinkage prior, useful for estimating sparse precision matrices with a **block-diagonal structure**.

Fiedler prior: motivation

Aim: take into account graph structure for prior specification.

Convenient way to capture connectivity of the graph: graph Laplacian .

Definition[Von Luxburg, 2007]: G undirected weighted graph, unnormalized Laplacian matrix \mathbf{L} is defined as $\mathbf{L} = \mathbf{D} - \mathbf{W}$, where

- weight matrix $\mathbf{W} = \{w_{ij}\}_{i,j=1}^p$, $w_{ij} \geq 0$
- degree matrix $\mathbf{D} = \text{diag}(\sum_j w_{1j}, \dots, \sum_j w_{pj})$

Properties of Laplacian \mathbf{L} with eigenvalues $\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_p$

- $\lambda_1 = 0$
- λ_2 is called Fiedler value or algebraic connectivity:
graph G is connected if and only if $\lambda_2 > 0$ (Fiedler regularization [Tam and Dunson, 2020])
- multiplicity k of the 0 eigenvalue of Laplacian equals to the number of connected components A_1, \dots, A_k [Von Luxburg, 2007].

Fiedler prior: definition

Consider partial correlation matrix $\mathbf{\Omega}$:

$$\mathbf{\Omega} = \{\omega_{ij}\}_{i,j=1}^p, \omega_{ij} \in [-1, 1] \text{ and } \omega_{ij} = -\Sigma_{ij}^{-1} / \sqrt{\Sigma_{ii}^{-1} \Sigma_{jj}^{-1}}.$$

Fiedler prior on $\mathbf{\Omega}$ with parameters $\boldsymbol{\delta} = (\delta_1, \dots, \delta_p)$, $\delta_j \geq 0$ is defined as

$$p(\mathbf{\Omega}|\boldsymbol{\delta}) = \frac{1}{Z(\boldsymbol{\delta})} \exp\left(-\sum_{j=1}^p \delta_j \lambda_j(\mathbf{\Omega})\right)$$

where:

- $L(|\mathbf{\Omega}|)$ - Laplacian matrix $|\mathbf{\Omega}|$
- $\lambda_1(\mathbf{\Omega}) \leq \dots \leq \lambda_p(\mathbf{\Omega})$ sorted eigenvalues of L .

To confront to precision matrix [Barnard et al., 2000]:

- $\Sigma^{-1} = \mathbf{T}\mathbf{\Omega}\mathbf{T}$, where $\mathbf{T} = \text{diag}(\tau_1, \dots, \tau_p)$.
- $\tau_j \stackrel{\text{iid}}{\sim} \text{Exp}(\eta)$, $j = 1, \dots, p$.

Fiedler prior: properties

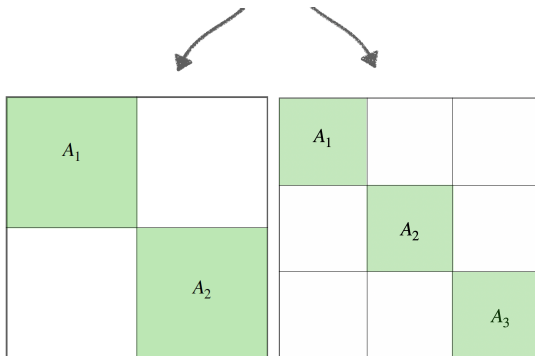
- By convention $\delta_1 = 0$
- if $\delta_2 = \dots = \delta_p = \delta^*$:

$$\sum_{i=1}^p \delta_i \lambda_i(\mathbf{\Omega}) = \delta^* \sum_{i=1}^p \lambda_i(\mathbf{\Omega}) = \delta^* \text{Tr}(L(|\mathbf{\Omega}|)) = \delta^* \sum_{i \neq j} |\omega_{ij}|$$

\implies Graphical Lasso for partial correlation matrices

Example:

$$\delta_2 > 0, \delta_3 = 0 \text{ or } \delta_2, \delta_3 > 0$$



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