Joint estimation of bipartite network collections. Application to plant-pollinator networks.

LSD

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Why a network?

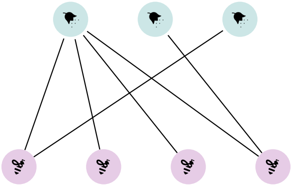

Figure 1: A toy network

$$\begin{pmatrix} 1 & 0 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 1 & 0 \end{pmatrix}$$

Associated bi-adjacency matrix

- Bipartite graph $G = (U, V, E)$
- Encoded in bi-adjacency matrix $Y \in \{0,1\}^{n_1 \times n_2}$

Why a network?

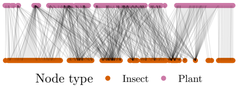

Figure 1: Plant-pollinator network from Bristol Baldock et al., 2019

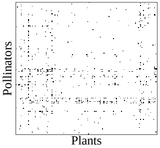

Figure 2: Adjacency matrix of the network

- Increasingly available
- Ecosystems described by their interactions
- Functional structure for: biodiversity monitoring, robustness, risk of collapse

Analysis methods for a network

Several methods :

- Metrics at
  - node level: degree, centrality. . .
  - network level: density, nestedness. . .

  Kolaczyk, 2009
- Node embedding and/or clustering with latent variable models
  Snijders and Nowicki, 1997; Hoff et al., 2002
- Node or network embedding with Graph Convolutional Networks
  Kipf and Welling, 2016

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Bipartite Stochastic Block Model (BiSBM[1])

Govaert and Nadif, 2005

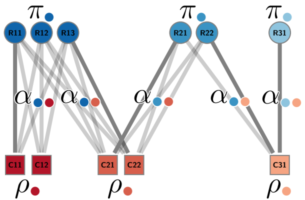

Figure 3: Example of BiSBM

Hierarchical model

$$\forall q \in [\![1, Q_1]\!], \mathbb{P}(Z_i = q) = \pi_q$$
$$\forall r \in [\![1, Q_2]\!], \mathbb{P}(W_j = r) = \rho_r$$
$$Y_{ij} | Z_i = q, W_j = r \sim \mathcal{B}ern(\alpha_{q,r})$$

where
$|\pi| = Q_1, |\rho| = Q_2, |\alpha| = Q_1 \times Q_2$

Concise BiSBM formula

$$Y \sim \mathcal{B}ern\text{-BiSBM}_{n_1,n_2}(Q_1, Q_2, \pi, \rho, \alpha)$$

[1] Commonly Known as *Latent Block Model* (LBM) in the literature.

How to compare multiple networks?

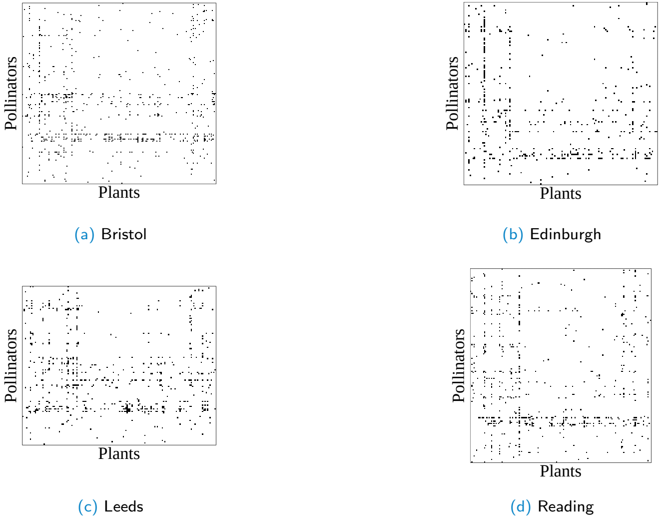

Figure 4: Adjacency matrices, Baldock et al., 2019

First approach: sep-BiSBM

$$\forall m \in \{1 \dots M\}, Y^m \overset{ind}{\sim} \mathcal{B}ern\text{-BiSBM}_{n_1^m, n_2^m}({Q_1}^m, {Q_2}^m, \pi^m, \rho^m, \alpha^m)$$

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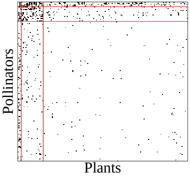
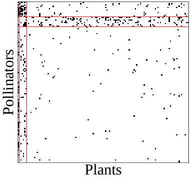
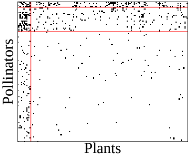


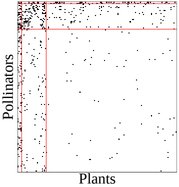
(a) Bristol, $Q_1 = 3$, $Q_2 = 3$



(b) Edinburgh, $Q_1 = 3$, $Q_2 = 3$



(c) Leeds, $Q_1 = 3$, $Q_2 = 2$



(d) Reading, $Q_1 = 3$, $Q_2 = 3$

Figure 5: Separate BiSBM fit for each network

Our contribution: joint models

iid-colBiSBM

$$\forall m \in \{1 \ldots M\}, Y^m \overset{iid}{\sim} \mathcal{B}ern\text{-BiSBM}_{n_1^m, n_2^m}(Q_1, Q_2, \pi, \rho, \alpha)$$

with $\theta = (\pi, \rho, \alpha)$.

- No shared nodes across networks
- Agnostic of structure

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$\pi\rho$-colBiSBM

$$\forall m \in \{1 \ldots M\}, Y^m \overset{ind}{\sim} \mathcal{B}ern\text{-BiSBM}_{n_1^m, n_2^m}(Q_1, Q_2, \pi^m, \rho^m, \alpha)$$

with $\theta = ((\pi^m)_{m=1,\ldots,M}, (\rho^m)_{m=1,\ldots,M}, \alpha)$.

- No shared nodes across networks
- Agnostic of structure

Parameter estimation

How ?

$$\ell(\mathbf{Y};\theta) = \sum_{m=1}^{M} \ell(Y^m;\theta)$$

$$= \sum_{m=1}^{M} \log \sum_{Z^m \in \mathcal{Z}^m, W^m \in \mathcal{W}^m} \exp\{\ell_c(Y^m, Z^m, W^m;\theta)\}$$

$$= \sum_{m=1}^{M} \log \sum_{Z^m \in \mathcal{Z}^m, W^m \in \mathcal{W}^m} \exp\{\ell(Y^m|Z^m, W^m;\alpha) + \ell(Z^m;\pi) + \ell(W^m;\rho)\}$$

Parameter estimation

How ?

$$
\begin{aligned}
\ell(\mathbf{Y};\theta) &= \sum_{m=1}^{M} \ell(Y^m;\theta) \\
&= \sum_{m=1}^{M} \log \sum_{Z^m\in\mathcal{Z}^m, W^m\in\mathcal{W}^m} \exp\{\ell_c(Y^m, Z^m, W^m;\theta)\} \\
&= \sum_{m=1}^{M} \log \sum_{Z^m\in\mathcal{Z}^m, W^m\in\mathcal{W}^m} \exp\{\ell(Y^m|Z^m, W^m;\alpha)+ \\
&\quad \ell(Z^m;\pi) + \ell(W^m;\rho)\}
\end{aligned}
$$

EM impracticable since $\mathbf{Z}, \mathbf{W}|\mathbf{Y}$ intractable due to conditional dependency.

Parameter estimation

Solution

Variational EM Daudin et al., 2008; Chabert-Liddell et al., 2024.

Variational approximation of $\mathbf{Z}, \mathbf{W} | \mathbf{Y}$

$\mathcal{R}_{Y^m,\tau}(Z^m, W^m) = \mathcal{R}^1_{\mathbf{Y}^m,\tau}(Z^m) \times \mathcal{R}^2_{\mathbf{Y}^m,\tau}(W^m) \Rightarrow$ independence between rows and columns, mean field approximation.

$$\ell(\mathbf{Y};\theta) \geq \sum_{m=1}^{M} \Big(\mathbb{E}_{\mathcal{R}_{Y^m,\tau}(Z^m,W^m)} [\ell_c(Y^m, Z^m, W^m; \theta)] + \mathcal{H}(\mathcal{R}_{Y^m,\tau}(Z^m, W^m)) \Big) =: \mathcal{J}(\mathcal{R}_{\mathbf{Y},\tau}; \theta)$$

where $\theta = (\pi, \rho, \alpha)$ for *iid*-colBiSBM

Selection criterion for Q_1, Q_2

Integrated Classification Likelihood (ICL) Biernacki et al., 2000

$$\begin{aligned}\mathrm{ICL}(\mathbf{Y}, Q_1, Q_2) &= \mathbb{E}_{\mathbf{Z},\mathbf{W}|\mathbf{Y}}[\ell_c(\mathbf{Y}, \mathbf{Z}, \mathbf{W}; \hat{\theta})] - \frac{1}{2}\mathrm{pen}(Q_1, Q_2) \\ &= \ell(\mathbf{Y}; \hat{\theta}) - \mathcal{H}(p(\mathbf{Z}, \mathbf{W}|\mathbf{Y}; \hat{\theta})) - \frac{1}{2}\mathrm{pen}(Q_1, Q_2)\end{aligned}$$

For SBM Daudin et al., 2008.

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For SBM Daudin et al., 2008.

$$\begin{aligned}\text{BIC-L}(\mathbf{Y}, Q_1, Q_2) &= \mathbb{E}_{\mathcal{R}_{\mathbf{Y},\hat{\tau}}}[\ell_c(\mathbf{Y}, \mathbf{Z}, \mathbf{W}; \hat{\theta}^{\mathrm{var}})] + \mathcal{H}(\mathcal{R}_{\mathbf{Y},\hat{\tau}}) - \frac{1}{2}\mathrm{pen}(Q_1, Q_2) \\ &= \mathcal{J}(\mathcal{R}_{\mathbf{Y},\hat{\tau}}, \hat{\theta}^{\mathrm{var}}) - \frac{1}{2}\mathrm{pen}(Q_1, Q_2)\end{aligned}$$

Practical problems of choosing Q_1, Q_2

Exploration problems

- Sensitivity to initializations.
- Exploration of a 2D grid is costly.

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- Sensitivity to initializations. $\rightarrow$ **Spectral clustering** and **split & merge** approach
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Practical problems of choosing Q_1, Q_2

Exploration problems

- Sensitivity to initializations. $\rightarrow$ **Spectral clustering** and **split & merge** approach
- Exploration of a 2D grid is costly. $\rightarrow$ **Greedy approach** and **sliding window**

Results Baldock et al., 2019

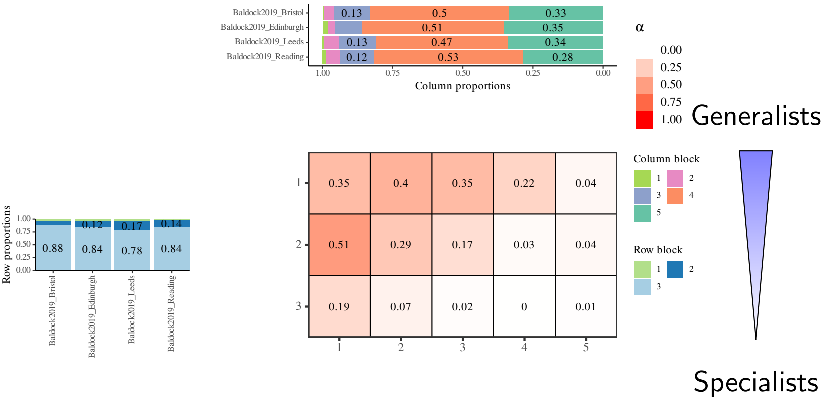
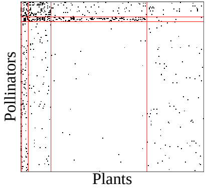
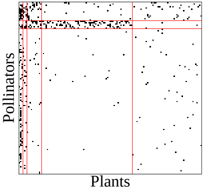


Figure 6: Shared structure (α matrix) and proportions (π and ρ) of the four networks

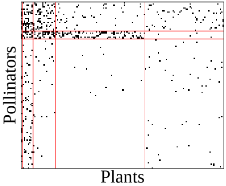
Results Baldock et al., 2019



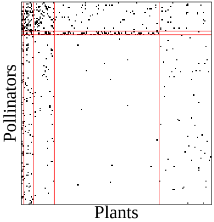
(a) Bristol



(b) Edinburgh



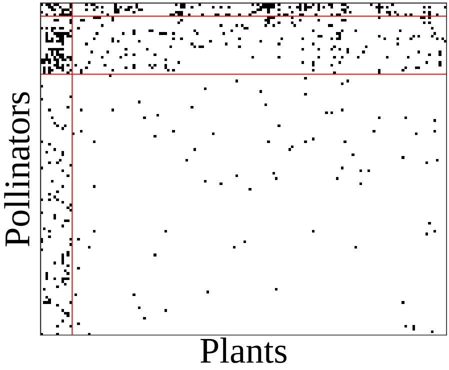
(c) Leeds



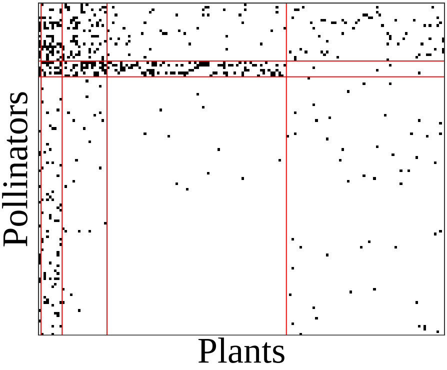
(d) Reading

Figure 6: *iid*-colBiSBM fit, $Q_1 = 3, Q_2 = 5$

Focus on Leeds



(a) sep-BiSBM, $Q_1 = 3, Q_2 = 2$



(b) *iid*-colBiSBM, $Q_1 = 3, Q_2 = 5$

Bombus

(a) *Bombus Hortorum* or garden bumblebee

(b) *Bombus Lapidarius* or red-tailed bumblebee

Bombus

(a) *Bombus Hortorum* or garden bumblebee

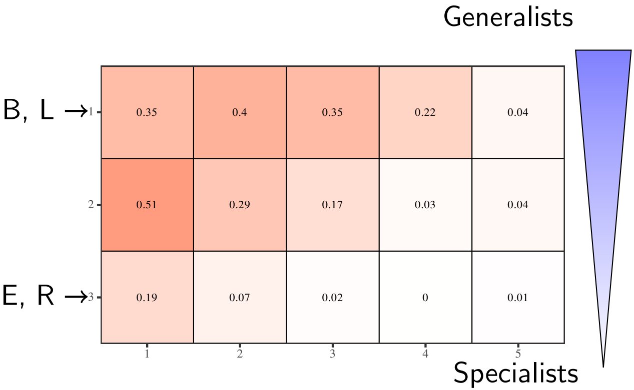


Figure 9: Shared structure (α matrix) of the four networks

Bombus

(b) *Bombus Lapidarius* or red-tailed bumblebee

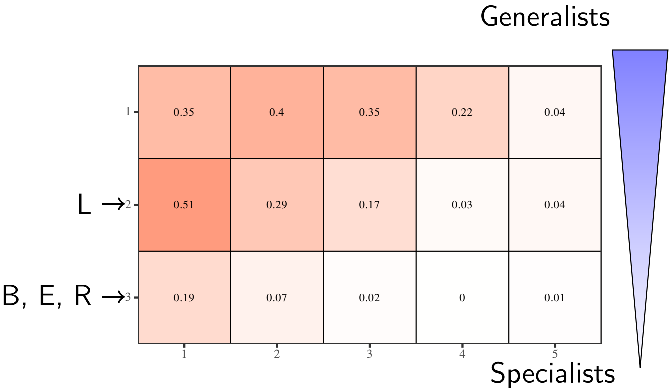


Figure 9: Shared structure (α matrix) of the four networks

Conclusion and perspectives

Summary

- 4 models including 3 flexible on at least one dimension (adaptability to data).
- Jointly detect classic and less classic structures agnostically.
- Partition a collection in sub-collections with homogeneous structures.
- R package `colSBM` at https://github.com/GrossSBM/colSBM

Future work

- Preprint in redaction
- Apply clustering to data from Pichon et al., 2024; Doré et al., 2021. Do interaction type drives the structure of the network?

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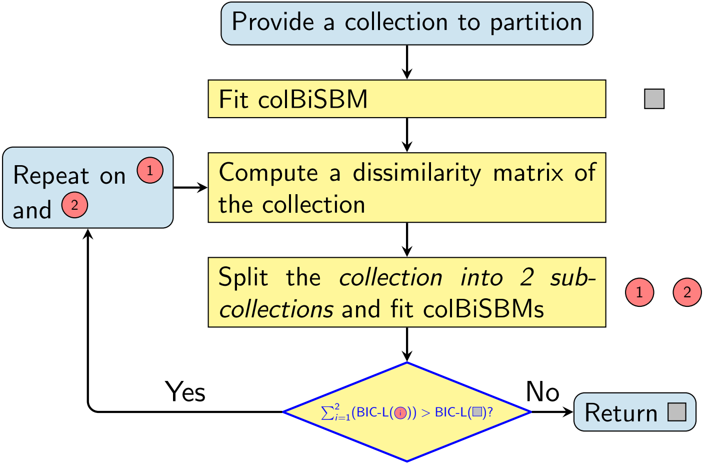
Clustering algorithm



$$D_{\mathcal{M}}(m, m') = \sum_{q=1}^{Q_1} \sum_{r=1}^{Q_2} \max(\widetilde{\pi}_q^m, \widetilde{\pi}_q^{m'}) \left(\widetilde{\alpha}_{qr}^m - \widetilde{\alpha}_{qr}^{m'}\right)^2 \max(\widetilde{\rho}_r^m, \widetilde{\rho}_r^{m'})$$

Developed formula of variational EM

$$\ell(\mathbf{Y};\theta) \geq \sum_{m=1}^{M} \Bigg(\sum_{i=1}^{n_1^m} \sum_{j=1}^{n_2^m} \sum_{q\in\mathcal{Q}_{1,m}} \sum_{r\in\mathcal{Q}_{2,m}} \tau_{i,q}^{1,m} \tau_{j,r}^{2,m} \log f(Y_{ij}^m;\alpha_{qr})$$
$$+ \sum_{i=1}^{n_1^m} \sum_{q\in\mathcal{Q}_{1,m}} \tau_{i,q}^{1,m} \log \pi_q{}^m + \sum_{j=1}^{n_2^m} \sum_{r\in\mathcal{Q}_{2,m}} \tau_{j,r}^{2,m} \log \rho_r{}^m$$
$$- \sum_{i=1}^{n_1} \tau_{i,q}^{1,m} \log \tau_{i,q}^{1,m} - \sum_{j=1}^{n_2} \tau_{j,r}^{2,m} \log \tau_{j,r}^{2,m} \Bigg) =: \mathcal{J}(\tau;\theta),$$

Variational approximation

$\tau_{iq}^{1,m} = \mathcal{R}^1_{Y^m,\tau}(Z_{iq}^m = 1)$ and $\tau_{jr}^{2,m} = \mathcal{R}^2_{Y^m,\tau}(W_{jr}^m = 1)$

Variational Expectation Step

$$\widehat{\tau}^{(t+1)} = \arg\max_{\tau} \mathcal{J}(\tau, \widehat{\boldsymbol{\theta}}^{(t)}) \Leftrightarrow \arg\min_{\tau \in \mathcal{T}} \mathbf{KL}[\mathcal{R}_{\mathbf{Y},\tau}, \mathbb{P}(.|\mathbf{Y})]$$

$$\begin{cases} \widehat{\tau}_{iq}^{1,m} \propto \widehat{\pi}_q^{m(t)} \prod_{j=1}^{n_2^m} \prod_{r \in \mathcal{Q}_2^m} f(Y_{ij}^m; \widehat{\alpha}_{qr}^{(t)})^{\widehat{\tau}_{jr}^{2,m(t+1)}} & \forall i = 1, \dots, n_1^m, q \in \mathcal{Q}_1^m \\ \widehat{\tau}_{jr}^{2,m} \propto \widehat{\rho}_r^{m(t)} \prod_{i=1}^{n_1^m} \prod_{q \in \mathcal{Q}_1^m} f(Y_{ij}^m; \widehat{\alpha}_{qr}^{(t)})^{\widehat{\tau}_{iq}^{1,m(t+1)}} & \forall j = 1, \dots, n_2^m, r \in \mathcal{Q}_2^m \end{cases}$$

[2] Initialization of $\widehat{\tau}$ with a *spectral clustering* on the networks.

Maximization Step

$$\widehat{\theta}^{(t+1)} = \arg\max_{\theta} \mathcal{J}(\widehat{\boldsymbol{\tau}}^{(t+1)}, \theta)$$

Connectivity parameters

$$\widehat{\alpha}_{qr} = \frac{\sum_{m=1}^{M} \sum_{i=1}^{n_1^m} \sum_{j=1}^{n_2^m} \tau_{iq}^{1,m} \tau_{jr}^{2,m} Y_{ij}^m}{\sum_{m=1}^{M} \sum_{i=1}^{n_1^m} \sum_{j=1}^{n_2^m} \tau_{iq}^{1,m} \tau_{jr}^{2,m}}$$

Proportions for *iid*

$$\widehat{\pi}_q = \frac{\sum_{m=1}^{M} \sum_{i=1}^{n_1^m} \tau_{iq}^{1,m}}{\sum_{m=1}^{M} n_1^m} \qquad \widehat{\rho}_r = \frac{\sum_{m=1}^{M} \sum_{j=1}^{n_2^m} \tau_{jr}^{2,m}}{\sum_{m=1}^{M} n_2^m}$$

Maximization Step

$$\widehat{\theta}^{(t+1)} = \arg\max_{\theta} \mathcal{J}(\widehat{\boldsymbol{\tau}}^{(t+1)}, \theta)$$

Connectivity parameters

$$\widehat{\alpha}_{qr} = \frac{\sum_{m=1}^{M} \sum_{i=1}^{n_1^m} \sum_{j=1}^{n_2^m} \tau_{iq}^{1,m} \tau_{jr}^{2,m} Y_{ij}^{m}}{\sum_{m=1}^{M} \sum_{i=1}^{n_1^m} \sum_{j=1}^{n_2^m} \tau_{iq}^{1,m} \tau_{jr}^{2,m}}$$

Proportions for $\pi \rho$

$$\widehat{\pi}^{m}{}_{q} = \frac{\sum_{i=1}^{n_1^m} \tau_{iq}^{1,m}}{n_1^m} \qquad \widehat{\rho}^{m}{}_{r} = \frac{\sum_{j=1}^{n_2^m} \tau_{jr}^{2,m}}{n_2^m}$$

Why does VE minimizes KL ?

$$\ell_c(\mathbf{Y},\mathbf{Z},\mathbf{W};\theta) = \log \mathbb{P}(\mathbf{Z},\mathbf{W}|\mathbf{Y};\theta) + \ell(\mathbf{Y};\theta)$$
$$\Leftrightarrow \ell(\mathbf{Y};\theta) = \ell_c(\mathbf{Y},\mathbf{Z},\mathbf{W};\theta) - \log \mathbb{P}(\mathbf{Z},\mathbf{W}|\mathbf{Y};\theta)$$
$$\Leftrightarrow \mathbb{E}_{\mathcal{R}_{\mathbf{Y},\tau}}[\ell(\mathbf{Y};\theta)] = \mathbb{E}_{\mathcal{R}_{\mathbf{Y},\tau}}[\ell_c(\mathbf{Y},\mathbf{Z},\mathbf{W};\theta)] - \mathbb{E}_{\mathcal{R}_{\mathbf{Y},\tau}}[\log \mathbb{P}(\mathbf{Z},\mathbf{W}|\mathbf{Y};\theta)]$$
$$\Leftrightarrow \ell(\mathbf{Y};\theta) = \mathbb{E}_{\mathcal{R}_{\mathbf{Y},\tau}}[\ell_c(\mathbf{Y},\mathbf{Z},\mathbf{W};\theta)] - \mathbb{E}_{\mathcal{R}_{\mathbf{Y},\tau}}[\log \mathbb{P}(\mathbf{Z},\mathbf{W}|\mathbf{Y};\theta)]$$

$$\text{But } \mathbf{KL}[\mathcal{R}_{\mathbf{Y},\tau}, \log \mathbb{P}(\mathbf{Z},\mathbf{W}|\mathbf{Y};\theta)] = -\mathbb{E}_{\mathcal{R}_{\mathbf{Y},\tau}}[\log \frac{\mathbb{P}(\mathbf{Z},\mathbf{W}|\mathbf{Y};\theta)}{\mathcal{R}_{\mathbf{Y},\tau}}]$$
$$= -\mathbb{E}_{\mathcal{R}_{\mathbf{Y},\tau}}[\log \mathbb{P}(\mathbf{Z},\mathbf{W}|\mathbf{Y};\theta)] + \underbrace{\mathbb{E}_{\mathcal{R}_{\mathbf{Y},\tau}[\log \mathcal{R}_{\mathbf{Y},\tau}]}}_{-\mathcal{H}(\mathcal{R}_{\mathbf{Y},\tau})}$$
$$\Leftrightarrow \mathbf{KL}[\mathcal{R}_{\mathbf{Y},\tau}, \log \mathbb{P}(\mathbf{Z},\mathbf{W}|\mathbf{Y};\theta)] + \mathcal{H}(\mathcal{R}_{\mathbf{Y},\tau}) = -\mathbb{E}_{\mathcal{R}_{\mathbf{Y},\tau}}[\log \mathbb{P}(\mathbf{Z},\mathbf{W}|\mathbf{Y};\theta)]$$

Thus $\ell(\mathbf{Y};\theta) - \mathbf{KL}[\mathcal{R}_{\mathbf{Y},\tau}, \log \mathbb{P}(\mathbf{Z},\mathbf{W}|\mathbf{Y};\theta)] = \mathcal{J}(\tau;\theta)$ □

On the BIC-L

$$\mathrm{ICL}(\hat{\theta}) = \mathbb{E}_{\mathbf{Z},\mathbf{W}|\mathbf{Y}}[\ell_c(\mathbf{Y},\mathbf{Z},\mathbf{W};\hat{\theta})] - \frac{1}{2}\mathrm{pen}(\dots)$$

$$\mathbb{E}_{\mathbf{Z},\mathbf{W}|\mathbf{Y}}[\ell_c(\mathbf{Y},\mathbf{Z},\mathbf{W};\hat{\theta})] = \log p(\mathbf{Y};\hat{\theta}) - \mathcal{H}(p(\mathbf{Z},\mathbf{W}|\mathbf{Y}))$$

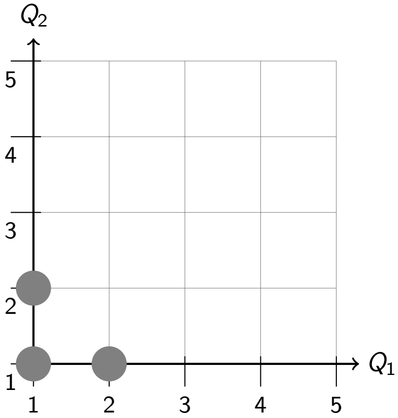
$$\text{And thus, } \mathrm{ICL}(\hat{\theta}) = \log p(\mathbf{Y};\hat{\theta}) - \mathcal{H}(p(\mathbf{Z},\mathbf{W}|\mathbf{Y})) - \frac{1}{2}\mathrm{pen}(\dots)$$

$\mathbf{Z},\mathbf{W}|\mathbf{Y}$ intractable, use the *variational approximation* $\mathcal{R}_{\mathbf{Y},\hat{\tau}}$ and don't penalize the entropy we derive the BIC-Like:

$$\mathrm{BIC\text{-}L}(\hat{\theta},\hat{\tau}) = \mathbb{E}_{\mathcal{R}_{\mathbf{Y},\hat{\tau}}}[\ell_c(\mathbf{Y},\mathbf{Z},\mathbf{W};\hat{\theta}^{\mathrm{var}})] + \mathcal{H}(\mathcal{R}_{\mathbf{Y},\hat{\tau}}) - \frac{1}{2}\mathrm{pen}(\dots)$$

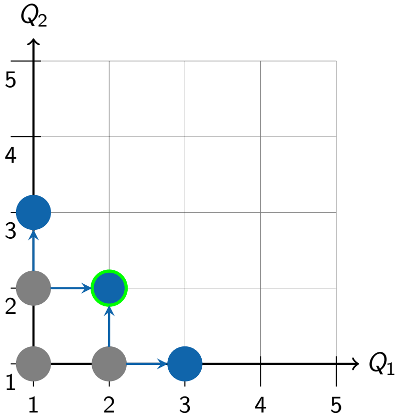
Biernacki et al., 2000; Daudin et al., 2008; Chabert-Liddell et al., 2024

Choice of (Q_1, Q_2) - Greedy approach



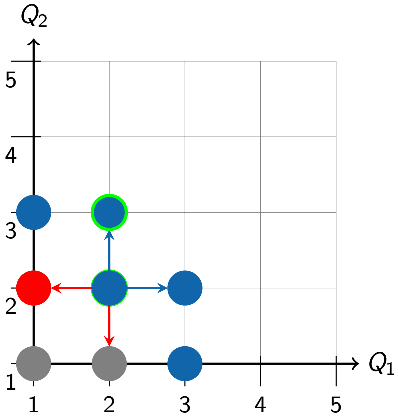
- Initial model :

Choice of (Q_1, Q_2) - Greedy approach



- Initial model :
- Model after *split* :
- Model maximizing the criterion :

Choice of (Q_1, Q_2) - Greedy approach



- Initial model :
- Model after *split* :
- Model maximizing the criterion :
- Model after *merge* :

Choice of (Q_1, Q_2) - Sliding window

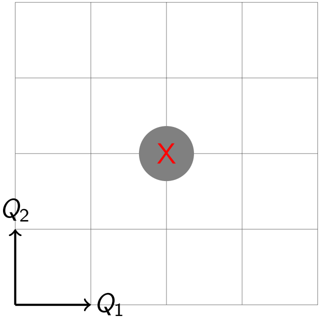


Figure 10: Sliding window

Choice of (Q_1, Q_2) - Sliding window

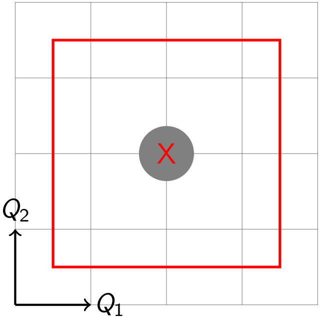


Figure 10: Sliding window

Choice of (Q_1, Q_2) - Sliding window

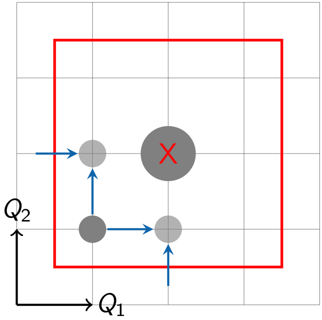


Figure 10: Sliding window

Initialization of the model if necessary

Choice of (Q_1, Q_2) - Sliding window

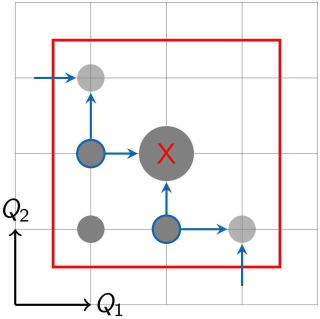


Figure 10: Sliding window

Choice of (Q_1, Q_2) - Sliding window

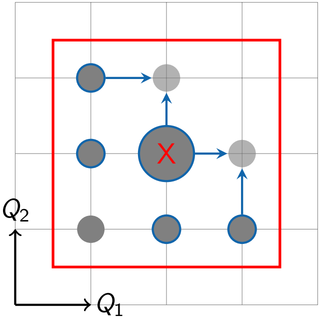


Figure 10: Sliding window

Choice of (Q_1, Q_2) - Sliding window

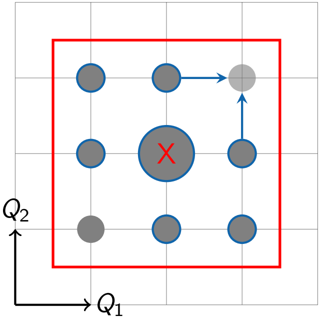


Figure 10: Sliding window

Choice of (Q_1, Q_2) - Sliding window

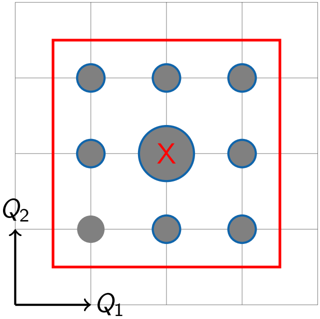


Figure 10: Sliding window

Choice of (Q_1, Q_2) - Sliding window

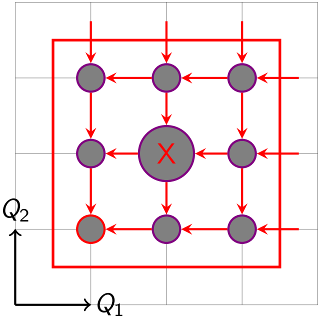


Figure 10: Sliding window

Choice of (Q_1, Q_2) - Sliding window

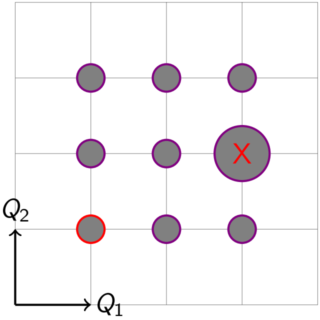


Figure 10: Sliding window

Localization of the new mode

Choice of (Q_1, Q_2) - Sliding window

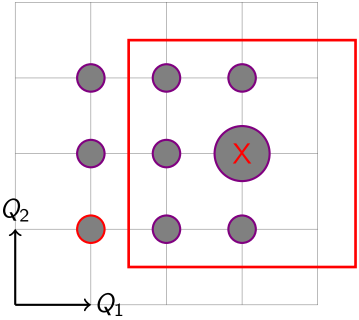


Figure 10: Sliding window

Move to the new mode then iterate

Figure 12: Map of the four cities

Appendices references I

Biernacki, C., Celeux, G., & Govaert, G. (2000). Assessing a mixture model for clustering with the integrated completed likelihood. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, *22*(7), 719–725. https://doi.org/10.1109/34.865189

Daudin, J.-J., Picard, F., & Robin, S. (2008). A mixture model for random graphs. *Statistics and Computing*, *18*(2), 173–183. https://doi.org/10.1007/s11222-007-9046-7

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