Rapport de stage dans l’UMR MIA Paris-Saclay

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Contents

Chapter 1

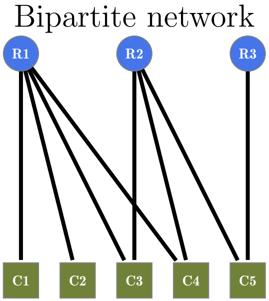
Présentation de l'UMR

Chapter 2

Context

2.1 Usage and importance of bipartite graphs

Bipartite graphs, denoted as $G = (U, V, E)$ with U and V two disjoint and independent sets of vertices and E the set of edges connecting U vertices to V vertices.



Incidence matrix

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

This representation can be used to represent various forms of interactions were two kinds of ”actors” interact. Those interactions can be binary or valued and a numeric representation is the incidence matrix, in the above example B.

Among the use case of bipartite graphs one can find the Netflix Problem, which was a prize organized by Netflix to improve its Recommender system. The row nodes are the movies and the columns are the user, at the intersection the value is the review of the user j for the movie i.

Another use is the representation of ecological interactions like plant-pollinator (Ramos-Jiliberto et al. 2010), birds-seed dispersion, prey-predator or host-parasite (Kaszewska-Gilas et al. 2021). In those cases, the rows are pollinator species and the columns are plant species, and the intersection is a value, binary if it is a presence/absence or a value if it is an abundance count.

Bipartite graphs are widely used in biology, in various fields, among which the previously cited ecological networks, but also in medicine with biomedical networks, biomolecular networks or epidemiological networks. (Pavlopoulos et al. 2018)

Some interesting results can arise when applying a tool widely used on a particular kind of interactions is used on another kind of interactions. Companies like Netflix use recommender system, to recommend another product to consumers based on their previous interactions. In Desjardins-Proulx et al. 2017 the authors use the *K-nearest neighbour* (KNN) algorithm as a Recommender to predict missing preys for predators in a predator-prey network.

2.2 Latent Block Model

The Latent Block Model (LBM) introduced by Gérard Govaert and Mohamed Nadif 2010 adapts the Stochastic Block Model (SBM) (Holland et al. 1983;Snijders and Nowicki 1997) to bipartite graphs.

Please note that we prefer the term ”BiSBM” and will use both LBM and BiSBM to designate the Stochastic Block model applied on bipartite networks.

This model supposes that:

- Row nodes are members of row blocks and column nodes are members of column blocks.
- The connectivity of two individuals is determined by their block memberships.
- An interaction can only occur between a row and a column node.

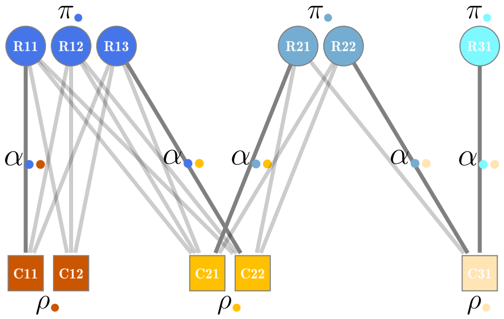


Figure 2.1: An LBM model visualization

On 2.1, π are the probabilities for a row node to belong to the row block of corresponding color, ρ are the probabilities for a column node to belong to the column block of corresponding color and α are the connectivity parameters between the row and column blocks.

This model can be used to easily generate bipartite graphs with complex and very varied structures. But when trying to determine the structure of a given network we need to find those parameters.

For this a common approach is to use a VEM algorithm (proposed for SBM in Daudin et al. 2008 and for LBM in G. Govaert and M. Nadif 2005) those groups and the required parameters can be inferred by maximizing a lower bound of the likelihood minus a penalty.

2.3 colSBM model, a joint model for a collection of networks

The *colSBM* model introduced by Chabert-Liddell et al. 2023 propose an extension of the SBM model to collections of SBMs. A collection is a set of networks which nodes are not common or linked between different networks, the interactions have the same valuations and are of the same type.

The model can retrieve the shared structure in a collection, indicate if networks should be grouped in a collection and in a large pool of networks, collections with common structures.

The next step after designing this collection model for unipartite was to adapt it to the bipartite case.

Chapter 3

Adjustment of colSBM to the bipartite case: colBiSBM

3.1 Definition of the model

Here are some common notations and conventions that we will use in the following sections.

3.1.1 A collection of i.i.d Bipartite SBM

As for *colSBM* this first model is the most constrained. It assumes that all the networks are the independent realizations of the same Q_1-Q_2-BiSBM with identical parameters. The *iid-colBiSBM* is defined as follows:

$$X^m \sim \mathcal{F} - BiSBM_{n_1,n_2}(Q_1, Q_2, \boldsymbol{\pi}, \boldsymbol{\rho}, \boldsymbol{\alpha}), \forall m = 1, \dots M, \tag{\textit{iid-colBiSBM}}$$

3.2 Variational Expectation step

Fixed point formula for the Bernoulli distribution:

- *iid* :

$$\begin{aligned}
\boldsymbol{\tau}^{m,1} &= {}^t\pi + \exp((\text{Mask}^m \odot A^m)\boldsymbol{\tau}^{m,2}\;{}^t(\text{logit}(\alpha)) + \text{Mask}^m\boldsymbol{\tau}^{m,2}\;{}^t\log(\mathbf{1} - \alpha)) \\
\boldsymbol{\tau}^{m,2} &= {}^t\rho + \exp(\;{}^t(\text{Mask}^m \odot A^m)\boldsymbol{\tau}^{m,1}\text{logit}(\alpha) + \;{}^t\text{Mask}^m\boldsymbol{\tau}^{m,1}\log(\mathbf{1} - \alpha))
\end{aligned}$$

- $\rho\pi$:

$$\begin{aligned}
\boldsymbol{\tau}^{m,1} &= {}^t\pi^m + \exp((\text{Mask}^m \odot A^m)\boldsymbol{\tau}^{m,2}\;{}^t(\text{logit}(\alpha)) + \text{Mask}^m\boldsymbol{\tau}^{m,2}\;{}^t\log(\mathbf{1} - \alpha)) \\
\boldsymbol{\tau}^{m,2} &= {}^t\rho^m + \exp(\;{}^t(\text{Mask}^m \odot A^m)\boldsymbol{\tau}^{m,1}\text{logit}(\alpha) + \;{}^t\text{Mask}^m\boldsymbol{\tau}^{m,1}\log(\mathbf{1} - \alpha))
\end{aligned}$$

with Mask^m the matrix containing 0 if the value is a NA and a 1 otherwise.

3.3 M step of the algorithm

Incorporate the equations from (Chabert-Liddell et al. 2023)

3.4 Computation of the variational bound

3.5 Penalties

iid-colBiSBM For the *iid-colBiSBM* the penalties were modified in the following way :

- For the πs and ρs:

$$\text{pen}_\pi(Q_1) = (Q_1 - 1)\log(\sum_{m=1}^{M} n_r^{(m)})$$

$$\text{pen}_\rho(Q_2) = (Q_2 - 1)\log(\sum_{m=1}^{M} n_c^{(m)})$$

- For the αs :

$$\text{pen}_\alpha(Q_1, Q_2) = Q_1 \times Q_2 \log(N_M)$$

  avec

$$N_M = \sum_{m=1}^{M} n_r^{(m)} \times n_c^{(m)}$$

And thus the BIC-L formula is now:

$$\text{BIC-L}(\boldsymbol{X}, Q_1, Q_2) = \max_{\theta} \mathcal{J}(\hat{\mathcal{R}}, \boldsymbol{\theta}) - \frac{1}{2}[\text{pen}_\pi(Q_1) + \text{pen}_\rho(Q_2) + \text{pen}_\alpha(Q_1, Q_2)]$$

$\rho\pi$-colBiSBM For the *$\rho\pi$-colBiSBM* the penalties are the following:

- The support penalties are:

$$\text{pen}_{S_1}(Q_1) = -2\log p_{Q_1}(S_1)$$

$$\text{pen}_{S_2}(Q_2) = -2\log p_{Q_2}(S_2)$$

  with

$$\log p_{Q_1}(S_1) = -M\log(Q_1) - \sum_{m=1}^{M} \log\binom{Q_1}{Q_1^{(m)}}$$

$$\log p_{Q_2}(S_2) = -M\log(Q_2) - \sum_{m=1}^{M} \log\binom{Q_2}{Q_2^{(m)}}$$

- Penalties for the ρs and πs:

$$\text{pen}_\pi(Q_1, S_1) = \sum_{m=1}^{M}(Q_1^{(m)} - 1)\log n_r^{(m)}$$

$$\text{pen}_\rho(Q_2, S_2) = \sum_{m=1}^{M}(Q_2^{(m)} - 1)\log n_c^{(m)}$$

- Penalties for the αs:

$$\text{pen}_\alpha(Q_1, Q_2, S_1, S_2) = (\sum_{q=1}^{Q_1}\sum_{r=1}^{Q_2}\mathbb{1}_{(S_1)'S_2>0})\log(N_M)$$

And the corresponding BIC-L formula:

$$\begin{aligned}\text{BIC-L}(\boldsymbol{X}, Q_1, Q_2) = \max_{S_1,S_2}[&\max_{\theta_{S_1,S_2}\in\Theta_{S_1,S_2}} \mathcal{J}(\hat{\mathcal{R}}, \theta_{S_1,S_2}) \\ &-\frac{1}{2}(\text{pen}_\pi(Q_1, S_1) + \text{pen}_\rho(Q_2, S_2) \\ &\quad + \text{pen}_\alpha(Q_1, Q_2, S_1, S_2) \\ &\quad + \text{pen}_{S_1}(Q_1) + \text{pen}_{S_2}(Q_2))]\end{aligned}$$

3.6 Latent space exploration and model selection

In order to explorer the bi-dimensional latent space (Q_1, Q_2) we use the following strategies.

3.6.1 Model selection

In the following steps the model selection consists of using the BIC-L criterion to select the model. We choose among the proposed models the one that maximizes the BIC-L

3.6.2 Initialization and pairing of the models

First to combine the information from the M networks we fit a collection model for each network at the two points $Q = (1, 2)$ and $Q = (2, 1)$. Using the previously described VEM algorithm we obtain for each network its parameters (ρ, π, α).

We then compute the marginal laws for each dimension, for each network. Then we order the network blocks by the probabilities obtained in decreasing order.

- For the memberships on the columns: $\mathit{col\ order}_m = \mathit{order}\,(\pi_m \times \alpha_m)$

- For the memberships on the rows: $\textit{row order}_m = \textit{order}\,(\rho_m \times\ ^t(\alpha_m))$

Using this order we relabel the memberships for the M fitted collection of a single network. Then we use the M memberships to fit a collection containing the M networks.

3.6.3 Greedy exploration to find an estimation of the mode

Using the previously fitted models for $Q = (1, 2)$ and $Q = (2, 1)$ we choose to perform a greedy exploration to find a first mode.

Meaning that for a given $Q = (Q_1, Q_2)$ we will compute all the possible memberships for the points $Q \in \{(Q_1+1, Q_2), (Q_1, Q_2+1), (Q_1-1, Q_2), (Q_1, Q_2-1)\}$, fit the corresponding models and choose the one that maximizes the BIC-L as the next point from which to repeat the procedure. We repeat the procedure until the BIC-L stops increasing 2 times in a row.

```
Input  : Fitted models for $Q = (1, 2)$ and $Q = (2, 1)$
Output: Estimation of the mode using greedy exploration

Initialize $Q = (1, 2)$ as the starting point Initialize BIC-L$_{\text{max}}$ as the
  maximum achieved BIC-L value Initialize $\textit{consecutive\_count}$ as 0

while $\textit{consecutive\_count} < 2$ do
    Compute possible memberships for
      $Q \in \{(Q_1 + 1, Q_2), (Q_1, Q_2 + 1), (Q_1 - 1, Q_2), (Q_1, Q_2 - 1)\}$;
    Fit models with the computed memberships Choose the model with
      the maximum BIC-L as the next point

    if $\textit{BIC-L} > \textit{BIC-L}_{max}$ then
        BIC-L$_{\text{max}}$ ← BIC-L $\textit{consecutive\_count}$ ← 0
    end
    else
        $\textit{consecutive\_count}$ ← $\textit{consecutive\_count} + 1$
    end

    $Q$ ← Next selected point
end

Output: Estimation of the mode using greedy exploration
```

Algorithm 1: Greedy Exploration for Mode Estimation

When this first estimation of the BIC-L mode has been find we apply the moving window on it.

3.6.4 Moving window to update the block memberships and the BIC-L

The *moving window* is used to update the block memberships on rows and columns and fit new models with those changes. To define the window, we use a center point and a *depth*, giving us the bottom left corner $(Q_{1,center} - depth, Q_{2,center} - depth)$ and the top right corner of the window $(Q_{1,center} + depth, Q_{2,center} + depth)$. All the points in this square will be updated and contribute to the update of the others. This procedure is repeated until convergence of the BIC-L.

The procedure consists of two alternating steps:

- the *forward pass*: repeatedly computing the possible splits to fit the current model.
- the *backward pass*: computing the possible merges to fit the current model.

```
Input  : Center point $(Q_{1,\text{center}}, Q_{2,\text{center}})$, depth
Output: Best model with maximum BIC-L in the window

Define bottom left corner $(Q_{1,\text{center}} - \text{depth}, Q_{2,\text{center}} - \text{depth})$
Define top right corner $(Q_{1,\text{center}} + \text{depth}, Q_{2,\text{center}} + \text{depth})$

while not converged do
    Forward pass:
    for $Q_1 \in [Q_{1,center} - depth; Q_{1,center} + depth]$ do
        for $Q_2 \in [Q_{2,center} - depth; Q_{2,center} + depth]$ do
            Compute possible splits from predecessors $(Q_1 - 1, Q_2)$ and
              $(Q_1, Q_2 - 1)$ Fit models with the block membership changes
              Compare and keep the best model based on BIC-L
        end
    end

    Backward pass:
    for $Q_1 \in [Q_{1,center} + depth; Q_{1,center} - depth]$ do
        for $Q_2 \in [Q_{2,center} + depth; Q_{2,center} - depth]$ do
            Compute possible merges from predecessors $(Q_1 + 1, Q_2)$ and
              $(Q_1, Q_2 + 1)$ Fit models with the block membership changes
              Compare and keep the best model based on BIC-L
        end
    end

    Update the best model based on the maximum BIC-L
end

Output: Best model with maximum BIC-L in the window
```

Algorithm 2: Moving Window Procedure

Forward pass The forward pass consists for a model at (Q_1, Q_2) to compute the possible splits from the block memberships of its ”predecessors”. The predecessors are the point at the left $(Q_1 - 1, Q_2)$ and below $(Q_1, Q_2 - 1)$ the current model (if they exist). To update the current model, we take its predecessors block

memberships and try to split one of the blocks in two. Then the current model is fitted using this clustering as a starting clustering. Once all the possible splits are fitted, they are compared, keeping the best, in the sense of the BIC-L. If a model was already present it is also compared and the best is chosen as the model for this round at (Q_1, Q_2).
The procedure then repeats for the point at (Q_1+1, Q_2) until it reaches $(Q_{1,center}+depth, Q_2)$ from which it repeats from $(Q_{1,center}-depth, Q_2+1)$. This repeats until computing the best model for $(Q_{1,center}+depth, Q_{2,center}+depth)$. *Note on the initialization:* The forward pass starts from the point $(Q_{1,center}+depth, Q_{2,center}+depth)$, so this points needs to have at least a model fitted. In the best case, the greedy exploration will have visited this point. But if the point has not been visited, a model will be fitted from a spectral initialization (i.e the block memberships is computed by using a spectral clustering). From this point, the next model will have at least one predecessor and the procedure can iterate.

Backward pass The backward pass consists for a model at (Q_1, Q_2) to compute the possible merges from the block memberships of its ”predecessors”. The predecessors are the point at the right (Q_1+1, Q_2) and on top (Q_1, Q_2+1) of the current model (if the predecessors exist). To update the current model, we take its predecessors block memberships and try to merge two blocks in one. Then the current model is fitted using this clustering as a starting clustering. Once all the possible merges are fitted, they are compared, keeping the best, in the sense of the BIC-L. If a model was already present it is also compared and the best is chosen as the model for this round at (Q_1, Q_2).
The procedure then repeats for the point at (Q_1-1, Q_2) until it reaches $(Q_{1,center}-depth, Q_2)$ from which it repeats from $(Q_{1,center}-depth, Q_2-1)$. This repeats until computing the best model for $(Q_{1,center}-depth, Q_{2,center}-depth)$. *Note on the initialization:* The backward pass starts from $(Q_{1,center}+depth, Q_{2,center}+depth)$, we know it was initialized at least by the forward pass, no special case here.

At the end of the moving window pass, the model of max BIC-L is the new best fit and the procedure can repeat until convergence.

3.7 Networks clustering

As in (Chabert-Liddell et al. 2023) we use a recursive algorithm to determine the best clustering of the given networks. The procedure being the same, only the technical modifications for the bipartite case will be explained below.

3.7.1 Distance between two networks

The distance weights uses π and ρ.

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

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List of Figures

List of Tables