SBM Laplace prior for concentration matrix

1 Model

Data: $X, i \in \{0, ..., n\}$ observations. $X \sim \mathcal{N}(0, \Sigma^{-1} = \Omega)$, Ω concentration matrix. Assumption: Q hidden clusters in the data. For each observation $i, Z_{iq} = \mathbb{1}_{i \in q}, q \in \{1, ..., Q\}$. $Z_{iq} = \text{independant latent variables}$.

- $\alpha_q = \mathbb{P}(i \in q)$ (Probability that observation i belongs to cluster q);
- $\sum_{q} \alpha_q = 1$;
- $Z_i \sim \mathcal{M}(1,\underline{\alpha})$ with $\underline{\alpha} = (\alpha_1,...,\alpha_Q)$ and $Z_i = (Z_{i1},...,Z_{iQ})$

Assumption:

$$\Omega_{ij}|\{Z_{iq}Z_{il}\}\sim Laplace(0,\lambda_{al}), (i,j)\in\{1,...,n\}^2, (q,l)\in\{1,...,Q\}^2$$

Laplace distribution:

$$\forall x \in \mathbb{R}, \ f_{ql}(x) = \frac{1}{2\lambda_{ql}} \exp{-\frac{|x|}{\lambda_{ql}}} \text{ if } q \neq l \text{ and } f_0x = \frac{1}{2\lambda_0} \exp{-\frac{|x|}{\lambda_0}} \text{ otherwise}$$

where $\lambda_{ql}, \lambda_0 > 0$ are scaling parameters and $\lambda_{ql} = \lambda_{lq}$. Λ matrix of parameters $\lambda_{ql}, (q, l) \in \{1, ..., Q\}^2$.

2 Complete likelihood

Assumptions reminder:

$$X|\Omega \sim \mathcal{N}(O, \Omega^{-1}), \quad \Omega|Z \sim Laplace(0, \Lambda), \quad Z \sim \mathcal{M}(1, \underline{\alpha})$$

Complete likelihood decomposition:

$$L_c(X, \Omega, Z) = \mathbb{P}(X, \Omega, Z)$$

$$= \mathbb{P}(X|\{\Omega, Z\})\mathbb{P}(\Omega|Z)\mathbb{P}(Z) \text{ conditional probabilities definition/formula}$$

$$= \mathbb{P}(X|\Omega)\mathbb{P}(\Omega|Z)\mathbb{P}(Z)$$

 $\mathbb{P}(X|\{\Omega,Z\}) = \mathbb{P}(X|\Omega)$, known distribution (knowing Z is equivalent to know Ω ?). Complete log-likelihood formula: (when $i \neq j$, otherwise replace λ_{ql} with λ_0)

$$\log L_{c}(X, \Omega, Z) = \log \mathbb{P}(X, \Omega, Z)$$

$$= \underbrace{\log \mathbb{P}(X|\Omega)}_{(1)} + \underbrace{\log \mathbb{P}(\Omega|Z)}_{(2)} + \underbrace{\log \mathbb{P}(Z)}_{(3)}$$

$$= \frac{n}{2} \left(\log(|\Omega|) - tr(S\Omega) - p\log(2\pi)\right) + \sum_{q,l,i,j,i\neq j} Z_{iq}Z_{jl} \left(-\log(2\lambda_{ql}) - \frac{|\Omega_{ij}|}{\lambda_{ql}}\right)$$

$$+ \sum_{i=1}^{n} \sum_{q=1}^{Q} Z_{iq} \log \alpha_{q}$$

Penalty term (lasso approach) in the article: $\sum_{q,l,i,j,i\neq j} Z_{iq} Z_{jl} \frac{|\Omega_{ij}|}{\lambda_{ql}}$. In the paper: notation $\|\rho_Z(\Omega)\|_{l_1}$.

(1):
$$X|\Omega \sim \mathcal{N}(0, \Omega^{-1})$$

Notation: $|\Omega| = det(\Omega) = 1/|\Omega^{-1}|$

$$\begin{split} \log \mathbb{P}(X|\Omega) &= \sum_{i=1}^n \log \left(\frac{1}{(2\pi)^{\frac{p}{2}} |\Omega^{-1}|} \exp(\frac{1}{2} x_i^T \Omega x_i) \right) \\ &= -\frac{n}{2} \left(p \log(2\pi) + \log(|\Omega^{-1}| \right) - \frac{1}{2} tr(X^T X \Omega) \\ &= -\frac{n}{2} \left(p \log(2\pi) - \log(|\Omega|) \right) - \frac{n}{2} tr(S\Omega) \text{ En notant } S = \frac{1}{n} X^T X \\ &= \frac{n}{2} \left(-p \log(2\pi) + \log(|\Omega|) \right) - \frac{n}{2} tr(S\Omega) \\ &= \frac{n}{2} \left(\log(|\Omega|) - tr(S\Omega) - p \log(2\pi) \right) \end{split}$$

(2):
$$\Omega|Z \sim Laplace(0,\Lambda)$$

Sophie : ici il faut changer tous les n en p = taille de Ω . If $i \neq j$:

$$\begin{split} \log \mathbb{P}(\Omega|Z) &= \log \prod_{i,j,q,l} \mathbb{P}(\Omega_{ij}|\{Z_{iq}Z_{jl}\})^{Z_{iq}Z_{jl}} \text{ Astuce termes puissance 0 ne participent pas au produit} \\ &= \sum_{\substack{q,l,i,j\\i\neq j}} Z_{iq}Z_{jl} \left(-\log(2\lambda_{ql}) - \frac{|\Omega_{ij}|}{\lambda_{ql}}\right) \\ &= -\sum_{\substack{q,l,i,j\\i\neq j}} Z_{iq}Z_{jl} \log(2\lambda_{ql}) - \sum_{\substack{q,l,i,j\\i\neq j}} Z_{iq}Z_{jl} \frac{|\Omega_{ij}|}{\lambda_{ql}} \\ \underbrace{\sum_{\substack{q,l,i,j\\i\neq j}}}_{\parallel \rho_Z(\Omega)\parallel_1} \end{split}$$

Otherwise:

$$\log \mathbb{P}(\Omega|Z) = \sum_{i} \left(-\log(2\lambda_0) - \frac{|\Omega_{ii}|}{\lambda_0} \right)$$

(3):
$$Z \sim \mathcal{M}(1,\underline{\alpha})$$

Sophie : ici il faut changer tous les n en p= taille de Ω .

$$\log \mathbb{P}(Z) = \log \prod_{i=1}^{n} \mathbb{P}(Z_i) = \log \prod_{i=1}^{n} \prod_{q=1}^{Q} \alpha_q^{Z_{iq}}$$
$$= \sum_{i=1}^{n} \sum_{q=1}^{Q} \log \alpha_q^{Z_{iq}} = \sum_{i=1}^{n} \sum_{q=1}^{Q} Z_{iq} \log \alpha_q$$

3 EM algorithm and variational estimation

Steps

- 1. Expectation (E): Calculate the expected value of the likelihood under the current parameters. Estimate Z_i , knowing Ω from previous step.
- 2. Maximization (M): Find parameters that maximizes the likelihood. Compute parameters knowing Z_i .

3.1 Definitions

Let \mathcal{Z} the space of all possibilities.

Definitions give us:

$$\log \mathbb{P}(Z|X,\Omega) = \log \mathbb{P}(X,\Omega,Z) - \log \mathbb{P}(X,\Omega)$$

3.2 E step: impossibility of direct computation and variational approach

In this part, Ω is known (as $\Omega^{(t)}$) from a previous M step. Considering $\mathbb{P}(X,\Omega)$ being constant with respect to Z:

$$\begin{split} \log \mathbb{P}(X,\Omega) &= \log \mathbb{P}(X,\Omega,Z) - \log \mathbb{P}(Z|X,\Omega) \\ &= \mathbb{E}_{Z|\Omega^{(t)}}[\log \mathbb{P}(X,\Omega,Z)] - \mathbb{E}_{Z|\Omega^{(t)}}[\log \mathbb{P}(Z|X,\Omega)] \\ &= \sum_{z \in \mathcal{Z}} \mathbb{P}(Z=z|\Omega^{(t)}) \log \mathbb{P}(X,\Omega,Z) - \sum_{z \in \mathcal{Z}} \mathbb{P}(Z=z|\Omega^{(t)}) \log \mathbb{P}(Z|X,\Omega) \\ &= \mathbb{E}_{Z|\Omega^{(t)}}[\log \mathbb{P}(X,\Omega,Z)] - \mathcal{H}(Z|X) \end{split}$$

The expected complete likelihood under the current parameters is:

$$\mathcal{Q}(\Omega|\Omega^{(t)}) = \mathbb{E}_{Z|\Omega^{(t)}}[\log \mathbb{P}(X,\Omega,Z)] = \sum_{z \in \mathcal{Z}} \mathbb{P}(Z=z|\Omega^{(t)}) \log \mathbb{P}(X,\Omega,Z)$$

 $\mathbb{P}(Z_{iq}Z_{jl}=1|\Omega_{ij}^{(t)})$ is unknown as Z_{iq} and Z_{jl} are not independent. Variational approach: take an approximation for $\mathbb{P}(Z|\Omega^t):=R_t(Z)$ for E step.

Now we consider the lower bond \mathcal{J} of $\mathbb{P}(X,\Omega)$:

$$\mathcal{J}_{\tau}(X, \Omega, R(Z)) := \log \mathbb{P}(X, \Omega) - D_{KL}\{R(Z) | | \mathbb{P}(Z|\Omega)\},\$$

where $D_{KL}\{R(Z)||\mathbb{P}(Z|\Omega)\}$ is the Küllback-Leibler divergence (i.e. distance between these two distributions). We take the following distribution for $R(.)^1$

$$R_{\tau}(Z) = \prod_{i=1}^{n} h_{\underline{\tau_i}}(Z_i),$$

where $h_{\underline{\tau_i}}$ is the density of the multinomial probability distribution $\mathcal{M}(1,\underline{\tau_i})$ and $\underline{\tau_i}=(\tau_{i1},...,\tau_{iQ})$ is a random vector containing the parmeters to optimize in the variational approach. Approximation of the probability that vertex i belongs to cluster q, τ_{iq} estimates $\mathbb{P}(Z_{iq}=1|\Omega)$, under the constraint $\sum_q \tau_{iq}=1$.

Küllback-Leibler divergence:

$$D_{KL}\{R_{\tau}(Z)||\mathbb{P}(Z|\Omega)\} = \sum_{Z \in \mathcal{Z}} R_{\tau}(Z) \log \frac{R_{\tau}(Z)}{\mathbb{P}(Z|\Omega)}$$
$$= \sum_{Z \in \mathcal{Z}} R_{\tau}(Z) \left(\log R_{\tau}(Z) - \log \mathbb{P}(Z|\Omega)\right)$$
$$= -\mathcal{H}(R_{\tau}(Z)) - \sum_{Z \in \mathcal{Z}} R_{\tau}(Z) \log \mathbb{P}(Z|\Omega)$$

New formula for the bound²:

$$\begin{split} \mathcal{J}_{\tau}(X,\Omega,R(Z)) &= \log \mathbb{P}(X,\Omega) - D_{KL}\{R(Z)||\mathbb{P}(Z|\Omega)\} \\ &= \log \mathbb{P}(X,\Omega) + \mathcal{H}(R_{\tau}(Z)) + \sum_{Z \in \mathcal{Z}} R_{\tau}(Z) \log \mathbb{P}(Z|\Omega) \\ &= \mathcal{H}(R_{\tau}(Z)) + \sum_{Z \in \mathcal{Z}} R_{\tau}(Z) \left(\log \mathbb{P}(Z|\Omega) + \log \mathbb{P}(X,\Omega) \right) \\ &= \mathcal{H}(R_{\tau}(Z)) + \underbrace{\sum_{Z \in \mathcal{Z}} R_{\tau}(Z) \log L_{c}(X,\Omega,Z)}_{\hat{Q}_{\tau}(\Omega) = \mathbb{E}_{\mathcal{R}_{\tau}}[\log \mathbb{P}(X,\Omega,Z)]} \end{split}$$

Objective: maximization of $\mathcal{J}(X,\Omega,R(Z))$.

 $^{^{1}}$ cf. Mariadassous and Robin, Uncovering latent structure in valued graphs: a variational approach, Technical Report 10, Statistics for Systems Biology, 2007

²En considérant que $\mathbb{P}(Z|\Omega) = \mathbb{P}(Z|\Omega,X)$ et en remarquant que $\log \mathbb{P}(X,\Omega)$ est indep de Z

Expression for $\hat{Q}_{\tau}(\Omega)$ Assume $R_{\tau}(Z) = \prod_{i=1}^{n} h_{\underline{\tau}_{i}}(Z_{i})$

$$\hat{Q}_{\tau}(\Omega) = \sum_{Z \in \mathcal{Z}} R_{\tau}(Z) \log L_c(X, \Omega, Z) = \mathbb{E}_{R_{\tau}} [\log L_c(X, \Omega, Z)]$$

$$= \frac{n}{2} (\log(|\Omega|) - tr(S\Omega) - p \log(2\pi)) + \sum_{i,j=1, j \neq i}^{n} \sum_{q,l=1}^{Q} \tau_{iq} \tau_{jl} \left(-\log(2\lambda_{ql}) - \frac{|\Omega_{ij}|}{\lambda_{ql}} \right) + \sum_{i=1}^{n} \sum_{q=1}^{Q} \tau_{iq} \log \alpha_q$$

Expression for $\mathcal{H}(R_{\tau}(Z))$ Assume $R_{\tau}(Z) = \prod_{i=1}^{n} h_{\underline{\tau_{i}}}(Z_{i})$

$$\mathcal{H}(R_{\tau}(Z)) = -\sum_{i=1}^{n} \sum_{q=1}^{Q} \mathbb{P}(Z_{iq} = 1) \log \mathbb{P}(Z_{iq} = 1)$$
$$= -\sum_{i=1}^{n} \sum_{q=1}^{Q} \tau_{iq} \log \tau_{iq}$$

Complete expression of $\mathcal{J}_{\tau}(X,\Omega,R(Z))$

$$\begin{split} \mathcal{J}_{\tau}(X,\Omega,R(Z)) &= \mathcal{H}(R_{\tau}(Z)) + \hat{Q}_{\tau}(\Omega) \\ &= \underbrace{\frac{n}{2} \left(\log(|\Omega|) - tr(S\Omega) - p \log(2\pi) \right)}_{\text{Constant par rapport à Z, et autres, désigné par c dans l'article} \\ &+ \sum_{\substack{i,j=1\\j\neq i}}^{n} \sum_{\substack{q,l=1}}^{Q} \tau_{iq} \tau_{jl} \left(-\log(2\lambda_{ql}) - \frac{|\Omega_{ij}|}{\lambda_{ql}} \right) + \sum_{i=1}^{n} \sum_{q=1}^{Q} \tau_{iq} \log \alpha_{q} - \sum_{i=1}^{n} \sum_{q=1}^{Q} \tau_{iq} \log \tau_{iq} \end{split}$$

Similar to the one in the complete likelihood expression, the penalty term is: $\sum_{i,j=1,j\neq i}^{n}\sum_{q,l=1}^{Q}\tau_{iq}\tau_{jl}\frac{|\Omega_{ij}|}{\lambda_{ql}}.$

3.3 E step: parameters estimation

Strategy: estimate τ_{iq} with fixed α_q and λ_{lq} , then estimate α_q and λ_{lq} considering $\hat{\tau}_{iq}$.

Estimating $\hat{\tau}_{iq}$: Introducing the constraint using Lagrange multiplier method. Constraint: $\sum_{q} \tau_{iq} = 1$.

$$\frac{\partial \mathcal{J}_{\tau}(X, \Omega, Z) - \lambda(\sum_{q=1}^{Q} \tau_{iq} - 1)}{\partial \tau_{iq}} = \sum_{\substack{j=1\\ i \neq i}}^{n} \sum_{l=1}^{Q} \tau_{jl} \left(-\log(2\lambda_{ql}) - \frac{|\Omega_{ij}|}{\lambda_{ql}} \right) + \log \alpha_q - 1 - \log \tau_{iq} - \lambda$$

$$\tau_{iq} = \exp\left[\sum_{\substack{j=1\\j\neq i}}^{n}\sum_{l=1}^{Q}\tau_{jl}\left(-\log(2\lambda_{ql}) - \frac{|\Omega_{ij}|}{\lambda_{ql}}\right) + \log\alpha_{q} - 1 - \lambda\right] = \exp(-1)\exp(-\lambda)\alpha_{q}\exp\left[\sum_{\substack{j=1\\j\neq i}}^{n}\sum_{l=1}^{Q}\tau_{jl}\left(-\log(2\lambda_{ql}) - \frac{|\Omega_{ij}|}{\lambda_{ql}}\right)\right]$$

$$= \exp(-1)\exp(-\lambda)\alpha_{q}\prod_{\substack{j=1\\j\neq i}}^{n}\prod_{l=1}^{Q}\exp\left[\tau_{jl}\left(-\log(2\lambda_{ql}) - \frac{|\Omega_{ij}|}{\lambda_{ql}}\right)\right] = \exp(-1)\exp(-\lambda)\alpha_{q}\prod_{\substack{j=1\\j\neq i}}^{n}\prod_{l=1}^{Q}\left(\frac{1}{2\lambda_{ql}}\exp\left(\frac{-|\Omega_{ij}|}{\lambda_{ql}}\right)\right)^{\tau_{jl}}$$

Using the constraint to find λ :

$$\sum_{q=1}^{Q} \tau_{iq} = 1 = \exp(-1) \exp(-\lambda) \alpha_q \prod_{\substack{j=1\\j\neq i}}^{n} \prod_{l=1}^{Q} \left(\frac{1}{2\lambda_{ql}} \exp\left(\frac{-|\Omega_{ij}|}{\lambda_{ql}}\right) \right)^{\tau_{jl}}$$

$$\Rightarrow \exp(\lambda) = \left[\sum_{q=1}^{Q} \exp(-1)\alpha_q \prod_{\substack{j=1\\j\neq i}}^{n} \prod_{l=1}^{Q} \left(\frac{1}{2\lambda_{ql}} \exp\left(\frac{-|\Omega_{ij}|}{\lambda_{ql}}\right) \right)^{\tau_{jl}} \right]^{-1}$$

$$\hat{\tau}_{iq} = \frac{\exp(-1)\alpha_q \prod_{\substack{j=1\\j\neq i}}^n \prod_{l=1}^Q \left(\frac{1}{2\lambda_{ql}} \exp\left(\frac{-|\Omega_{ij}|}{\lambda_{ql}}\right)\right)^{\tau_{jl}}}{\sum_{\substack{q=1\\q\neq i}}^Q \exp(-1)\alpha_q \prod_{\substack{j=1\\j\neq i}}^n \prod_{l=1}^Q \left(\frac{1}{2\lambda_{ql}} \exp\left(\frac{-|\Omega_{ij}|}{\lambda_{ql}}\right)\right)^{\tau_{jl}}}$$

In the paper:

$$\widehat{\tau}_{iq} \propto \alpha_q \prod_{\substack{j=1\\j\neq i}}^n \prod_{l=1}^Q \left(\frac{1}{2\lambda_{ql}} \exp\left(\frac{-|\Omega_{ij}|}{\lambda_{ql}}\right)\right)^{\tau_{jl}}$$

Estimating $\hat{\alpha}_q$: With constraint $\sum_q \alpha_q = 1$.

$$\left. \frac{\partial \mathcal{J}_{\tau}(X, \Omega, Z)}{\partial \alpha_q} \right|_{\tau_{iq}} = \sum_{i=1}^n \sum_{q=1}^Q \tau_{iq} \frac{1}{\alpha_q}$$

The value if α_q will be derived from the following expression:

$$\left. \frac{\partial \mathcal{J}_{\tau}(X, \Omega, Z) - \eta(\sum_{q} \alpha_{q} - 1)}{\partial \alpha_{q}} \right|_{\tau_{iq}} = \sum_{i=1}^{n} \tau_{iq} \frac{1}{\alpha_{q}} - \eta$$

$$0 = \sum_{i=1}^{n} \tau_{iq} \frac{1}{\alpha_{q}} - \eta \Leftrightarrow \alpha_{q} = \frac{\sum_{i} \tau_{iq}}{\eta}$$
$$\Leftrightarrow \sum_{q} \alpha_{q} = \frac{\sum_{q} \sum_{i} \tau_{iq}}{\eta} \Leftrightarrow 1 = \frac{n}{\eta} \Leftrightarrow \boxed{\eta = n}$$
$$0 = \sum_{i=1}^{n} \tau_{iq} \frac{1}{\alpha_{q}} - \eta \Leftrightarrow \alpha_{q} = \frac{\sum_{i}^{n} \tau_{iq}}{\eta}$$

$$\hat{\alpha}_q = \frac{\sum_{i=1}^{n} \tau_{iq}}{n}$$

Estimating $\hat{\lambda}_{lq}$:

$$\left. \frac{\partial \mathcal{J}_{\tau}(X, \Omega, Z)}{\partial \lambda_{ql}} \right|_{\tau_{iq}} = \sum_{\substack{j=1\\ j \neq i}}^{p} \tau_{iq} \tau_{jl} \left(-\frac{1}{2\lambda_{ql}} + \frac{|\Omega_{ij}|}{\lambda_{ql}^{2}} \right)$$

$$0 = \sum_{\substack{j=1\\j\neq i}}^{p} \tau_{iq} \tau_{jl} \left(-\frac{1}{2\lambda_{ql}} + \frac{|\Omega_{ij}|}{\lambda_{ql}^2} \right)$$

$$\Rightarrow 0 = \sum_{\substack{j=1\\j\neq i}}^{p} \tau_{iq} \tau_{jl} \left(-\frac{1}{2} + \frac{|\Omega_{ij}|}{\lambda_{ql}} \right)$$

$$\hat{\lambda}_{ql} = \frac{\sum_{\substack{j=1\\j\neq i}}^{n} \tau_{iq} \tau_{jl} |\Omega_{ij}|}{\sum_{\substack{j=1\\j\neq i}}^{n} \tau_{iq} \tau_{jl}}$$

4 Likelihood penalized point of view

Maybe talking of "model" like in Section 1 is not a good idea. We should consider the penalized likelihood approach.

Inference of graphical model with prior point of view Originally, to estimate Ω , it is standard to consider the lasso penalization

$$= \log \mathbb{P}(X|\Omega) - \lambda^{-1} \sum_{i < j} |\Omega_{ij}| - \lambda_0^{-1} \sum_{i=1}^p |\Omega_{ii}|$$
$$\widehat{\Omega}_{\lambda} = \arg \max_{\Omega} \mathcal{S}(X, \Omega, \lambda)$$

We see that:

$$\lambda^{-1} \sum_{i < j} |\Omega_{ij}| = \sum_{i < j} \log \exp\left(-\frac{\|\Omega\|}{\lambda}\right)$$

$$= \sum_{i < j} \log\left(\frac{1}{2\lambda} \exp\left(-\frac{|\Omega_{ij}|}{\lambda}\right)\right) + \sum_{i < j} \log(2\lambda)$$

$$= \log \mathbb{P}(\Omega; \lambda) + Cste(\lambda) + \frac{p(p-1)}{2} \log(\lambda)$$

where $\mathbb{P}(\Omega; \lambda)$ is the prior such that the

$$\Omega_{ij} \sim_{i.i.d} Laplace(0, \lambda), \quad i < j, \text{ and } \quad \Omega_{ii} \sim_{i.i.d} Laplace(0, \lambda_0),$$

normalized over the precision matrices that are positive definite (meaning that we set a null prior on the non positive definite matrices Ω). More precisely, let \mathcal{D} be the positive definite matrices, we set:

$$\mathbb{P}(\Omega; \lambda) = \frac{\mathbf{1}_{\Omega \in \mathcal{D}} \prod_{i < j} \lambda e^{-\lambda |\Omega_{ij}|} \prod_{i} \lambda_0 e^{-\lambda_0 |\Omega_{ii}|}}{\int \mathbf{1}_{\Omega \in \mathcal{D}} \prod_{i < j} \lambda e^{-\lambda |\Omega_{ij}|} \prod_{i} \lambda_0 e^{-\lambda_0 |\Omega_{ii}|} d\Omega}$$

If λ is known, then the denominator of $\mathbb{P}(\Omega;\lambda)$ does not depend on Ω and so:

$$\begin{split} \widehat{\Omega}_{\lambda} &= \arg \max_{\Omega} \mathcal{S}(X, \Omega, \lambda) \\ &= \arg \max_{\Omega} \ \log \mathbb{P}(X | \Omega) + \log \mathbb{P}(\Omega; \lambda) + Cste(\lambda) \\ &= \arg \max_{\Omega} \ \log \mathbb{P}(X | \Omega) + \log \mathbb{P}(\Omega; \lambda) \\ &= \arg \max_{\Omega} \ \mathbb{P}_{\lambda}(\Omega | X) \end{split}$$

where $\mathbb{P}_{\lambda}(\Omega|X)$ is the posterior distribution corresponding to the prior distribution $\mathbb{P}(\Omega;\lambda)$

A different prior distribution on Ω Now we propose to change the prior distribution :

We set a SBM prior on Ω . We fix K the number of clusters

$$Z_{i} \sim i.i.d.\mathcal{M}(1,\pi) \quad \forall i \in \{1,\ldots,p\}$$

$$\Omega_{ij}|Z_{i} = k, Z_{j} = \ell \sim Laplace(\lambda_{k\ell}) \quad \forall i < j \in \{1,\ldots,p\}$$

$$\Omega_{ii} \sim Laplace(\lambda_{0}) \quad \forall i \in \{1,\ldots,p\}$$

But, to consider the "prior" point of view, we have to restrict this prior over the definite positive matrices

$$\mathbb{P}_{\pi,\lambda,K,\mathcal{D}}(\Omega) \propto \mathbf{1}_{\Omega \in \mathcal{D}} \sum_{\mathbf{Z}} P(\Omega|\mathbf{Z};\lambda) P(\mathbf{Z};\pi) = \frac{\mathbf{1}_{\Omega \in \mathcal{D}} \sum_{\mathbf{Z}} P(\Omega|\mathbf{Z};\lambda) P(\mathbf{Z};\pi)}{\int \mathcal{D} \sum_{\mathbf{Z}} P(\Omega|\mathbf{Z};\lambda) P(\mathbf{Z};\pi) d\Omega}$$

If K, λ and π are know then we have to optimize:

$$\widehat{\Omega}_{\pi,\lambda,K} = \arg \max_{\Omega} \mathcal{S}(X,\Omega,\lambda,\pi,K)$$

$$\mathcal{S}(X,\Omega,\lambda,\pi,K) = \log \mathbb{P}(X|\Omega) + \log \mathbb{P}_{\pi,\lambda,K,\mathcal{D}}(\Omega;\theta)$$

However, that way, we have to optimize Ω under the constraint...

An other strategy similar to the one proposed by [1] or [2] is to remove the constraint from the prior and maximise a pseudo-likelihood. More precisely:

$$\widehat{\Omega}_{\lambda} = \arg \max_{\Omega} \widetilde{\mathcal{S}}(X, \Omega, \lambda)$$

with

$$\widetilde{\mathcal{S}}(X, \Omega, \lambda, \pi, K) = \log \widetilde{\mathcal{S}}(X|\Omega) + \log \mathbb{P}_{\pi, \lambda, K}(\Omega)$$

where

$$\mathbb{P}_{\pi,\lambda,K}(\Omega) = \sum_{\mathbf{Z}} P(\Omega|\mathbf{Z};\lambda) P(\mathbf{Z};\pi)$$

and $\log \widetilde{\mathcal{S}}(X|\Omega)$ is the linear regression version of the Ω_{ij} .

New strategy An other strategy could be to put a SBM prior distribution on the Ω_{ij} (i < j) and set $\Omega_{ii} = \sum_{j \neq i} \Omega_{ij}$ In that case, the matrix Ω automatically becomes positive definite. It could be any other transformation making the matrix inversible.

So let us define: Ω_T the upper triangular coefficients of Ω . We set a prior SBM distribution on Ω_T . Ω is deduced deterministically from Ω_T . We denote by Φ this deterministic function.

We set:

$$\widetilde{\widetilde{\mathcal{S}}}(X,\Omega_T,\lambda,\Omega,\lambda,\pi,K) = \log \mathbb{P}(X|\Phi(\Omega_T)) + \log \mathbb{P}_{\pi,\lambda,K}(\Omega_T)$$

We want to optimize it with respect to Ω_T and π, λ (for a fixed K). We won't be able to do it because $\log \mathbb{P}_{\pi,\lambda,K}(\Omega_T)$ has no explicit expressions. We introduced a lower bound of $\widetilde{\widetilde{\mathcal{S}}}(X,\Omega_T,\lambda,\Omega,\lambda,\pi,K)$, namely $\mathcal{J}(X,\Omega_T,\lambda,\Omega,\lambda,\pi,K,\tau)$

$$\mathcal{J}_{K}(X; \Omega_{T}, \lambda, \pi, \tau) = \log \mathbb{P}(X|\Phi(\Omega_{T})) + \log \mathbb{P}_{\pi, \lambda, K}(\Omega_{T}) - \mathcal{K}(\mathcal{R}_{\tau}, P(Z|\Omega))
= \log \mathbb{P}(X|\Phi(\Omega_{T})) + \mathbb{E}_{\mathcal{R}_{\tau}}[\log P(\Omega_{T}, \mathbf{Z}; \lambda, \pi)] + \mathcal{H}(\mathcal{R}_{\tau}(\cdot))$$

We can optimize it iteratively. At iteration t.

1.

$$(\pi^{(t)}, \lambda^{(t)}) = \arg \max_{\pi \lambda} \mathcal{J}_K(X; \Omega_T^{(t-1)}, \lambda, \pi, \tau^{(t-1)})$$

It is the M-step of the VEM.

2.

$$\tau^{(t)} = \arg\max_{\tau} \mathcal{J}_K(X; \Omega_T^{(t-1)}, \lambda^{(t)}, \pi^{(t)}, \tau)$$

It the E-step of the VEM. Resulting into a fixed point equation. We could also use a lower bound of this preventing from resolving a fixed point equation (GEM).

3.

$$\Omega_{T}^{(t)} = \arg \max_{\Omega_{T}} \log \mathbb{P}(X|\Phi(\Omega_{T})) + \mathbb{E}_{\mathcal{R}_{\tau^{(t)}}} \left[\log P(\Omega_{T}, \mathbf{Z}; \lambda^{(t)}, \pi^{(t)}) \right] + \mathcal{H}(\mathcal{R}_{\tau^{(t)}}(\cdot))$$

$$= \arg \max_{\Omega_{T}} \left[\log \mathbb{P}(X|\Phi(\Omega_{T})) + \sum_{i < j} \sum_{k,l} \tau_{ik}^{(t)} \tau_{j\ell}^{(t)} (\log \lambda_{k,\ell}^{(t)} - \lambda_{k\ell}^{(t)} |\Omega_{ij}|) \right]$$

$$= \arg \max_{\Omega_{T}} \left[\log \mathbb{P}(X|\Phi(\Omega_{T})) - \sum_{i < j} \sum_{k,l} \tau_{ik}^{(t)} \tau_{j\ell}^{(t)} \lambda_{k\ell}^{(t)} |\Omega_{ij}| \right]$$

I state that it is equivalent to estimating Ω in its complete version (upper and diagonal) under the constraint $\Omega_{ii} = \sum_{i \neq j} \Omega_{ij}$ which is a linear constraint:

$$\Omega_{ii} - \sum_{i \neq j} \Omega_{ij} = 0$$

Using a Lagrange approach, we get:

$$\Omega^{(t)} = \arg \max_{\Omega} \left[\log \mathbb{P}(X|\Omega) - \sum_{i < j} \sum_{k,l} \tau_{ik}^{(t)} \tau_{j\ell}^{(t)} \lambda_{k\ell}^{(t)} |\Omega_{ij}| \right] + \sum_{i=1}^{p} \nu_i \left(\Omega_{ii} - \sum_{i \neq j} \Omega_{ij} \right)$$

And $\Omega_T^{(t)}$ is the upper triangular part of $\Omega^{(t)}$ Is it feasible Julien ????

References

- [1] Benjamin M. Marlin and Kevin P. Murphy. Sparse Gaussian graphical models with unknown block structure. pages 1–8, 2009.
- [2] Siqi Sun and Hai Wang. Inferring Block Structure of Graphical Models in Exponential Families. Proceedings of the 18th International Conference on Artifical Intelligence and Statistics (AISTATS) International Conference on Machine Learning ICML '09, 38, 2015.