SBM for reconstructed network

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1 Introduction

2 Model

Data

- $p \text{ nodes} = \text{species } (1 \le i, j \le n)$
- K clusters $(1 \le k, \ell \le K)$
- Z_i = cluster of node i, $Z_{ik} = \mathbb{I}\{Z_i = k\}$, $Z = (Z_i)$
- $G_{ij} = \mathbb{I}\{i \sim k\} = \text{connection between nodes } i \text{ and } j, G = (G_{ij}) = \text{unobserved network}$
- S_{ij} = score of edge between nodes i and j, $S = (S_{ij})$ = observed score matrix

Parameters

- $\pi = (\pi_k) = \text{cluster proportions}$
- $\gamma = (\gamma_{k\ell})$ = between cluster connection probabilities
- ψ_0 = parameter of the score distribution for absent edge $p(S_{ij} \mid G_{ij} = 0)$ (idem ψ_1 for present edge), $\psi = (\psi_0, \psi_1)$
- $\theta = (\pi, \gamma, \psi)$

Model

• (Z_i) iid,

$$Z_i \sim \mathcal{M}(1,\pi)$$

• (G_{ij}) independent conditionally on Z,

$$(G_{ij} \mid Z_i = k, Z_j = \ell) \sim \mathcal{B}(\gamma_{k\ell})$$

• (S_{ij}) independent conditionally on G,

$$(S_{ij} \mid G_{ij} = u) \sim F(\cdot; \psi_u), \qquad u = 0, 1$$

We further denote $F_u(\cdot) = F(\cdot; \psi_u)$ and $f_u(\cdot)$ the corresponding pdf.

Properties and definitions

• S and Z independent conditionally on G:

$$p(Z \mid G, S) = p(Z \mid G), \qquad p(S \mid G, Z) = p(S \mid G)$$

• Distribution of G_{ij}

$$P(G_{ij} = 1 \mid S_{ij}, Z_i = k, Z_j = \ell) = \frac{\gamma_{k\ell} f_1(S_{ij})}{\gamma_{k\ell} f_1(S_{ij}) + (1 - \gamma_{k\ell}) f_0(S_{ij})} =: \eta_{ij}^{k\ell} \widetilde{P}(G_{ij} = 1 \mid S_{ij}) = \sum_{k,\ell} \tau_{ik} \tau_{j\ell} \eta_{ij}^{k\ell} =: \overline{\eta}_{ij}$$

• Kullback-Leibler divergence

$$\begin{split} KL(q(U); p(U)) &= \mathbb{E}_q(\log q(U) - \log p(U)) \\ KL(q(U, V); p(U, V)) &= \mathbb{E}_{q(U, V)}(\log q(U) + \log(q(V \mid U) - \log p(U) - \log p(V \mid U)) \\ &= KL(q(U); p(U)) + \mathbb{E}_{q(U)}KL(q(V \mid U), p(V \mid U)) \end{split}$$

3 Inference

3.1 Loss function

Log-likelihood

$$\log p(Z, G, S) = \log p(Z; \pi) + \log p(G \mid Z; \gamma) + \log p(S \mid G; \psi)$$

$$= \sum_{i,k} Z_{ik} \log \pi_k + \sum_{i < j} \sum_{k,\ell} Z_{ik} Z_{j\ell} (G_{ij} \log \gamma_{k\ell} + (1 - G_{ij}) \log (1 - \gamma_{k\ell}))$$

$$+ \sum_{i < j} G_{ij} \log f_1(S_{ij}) + (1 - G_{ij}) \log f_0(S_{ij})$$

Approximate distribution $q(Z,G) \approx p(Z,G \mid S)$

$$q(Z,G) = q(Z)q(G \mid Z) := q(Z)p(G \mid Z,S)$$

$$\tag{1}$$

where

$$p(G \mid Z, S) = \prod_{i,j} p(G_{ij} \mid Z_i, Z_j, S_{ij})$$

and

$$q(Z) = \prod_{i} q_i(Z_i) = \prod_{i,k} \tau_{ik}^{Z_{ik}}.$$

Divergence $KL(q(Z,G); p(Z,G \mid S))$

$$KL(q(Z,G);p(Z,G\mid S)) = KL(q(Z)p(G\mid Z,S);p(Z\mid S)p(G\mid Z,S))$$

$$= KL(q(Z);p(Z\mid S)) + \mathbb{E}_{q(Z)}\underbrace{KL(p(G\mid Z,S);p(G\mid Z,S))}_{=0}$$

Still, the conditional entropy of $q(G \mid Z)$ contributes to the lower bound.

Lower bound $J(\theta, q)$

$$J(\theta, q) = \log p_{\theta}(S) - KL(q(Z, G); p(Z, G \mid S))$$

$$= \mathbb{E}_{q} \log p_{\theta}(Z, G, S) + H(q(Z)) + \mathbb{E}_{q}H(q(G \mid Z))$$

$$= \sum_{i,k} \tau_{ik} \log \pi_{k} + \sum_{i < j} (\overline{\eta}_{ij} \log \gamma_{k\ell} + (1 - \overline{\eta}_{ij}) \log(1 - \gamma_{k\ell}))$$

$$+ \sum_{i < j} \sum_{k,\ell} \tau_{ik} \tau_{j\ell} (\eta_{ij}^{k\ell} \log f_{1}(S_{ij}) + (1 - \eta_{ij}^{k\ell}) \log f_{0}(S_{ij}))$$

$$- \sum_{i,k} \tau_{ik} \log \tau_{ik} - \sum_{i < j} \sum_{k,\ell} \tau_{ik} \tau_{j\ell} (\eta_{ij}^{k\ell} \log \eta_{ij}^{k\ell} + (1 - \eta_{ij}^{k\ell}) \log(1 - \eta_{ij}^{k\ell}))$$
(3)

3.2 Estimation equation

VE step Denoting

$$\log A_{ijk\ell} = \eta_{ij}^{k\ell} (\log \gamma_{k\ell} + \log f_1(S_{ij})) + (1 - \eta_{ij}^{k\ell}) (\log(1 - \gamma_{k\ell}) + \log f_0(S_{ij}))$$

setting the derivative wrt τ_{ik} to zero with the contraint $\sum_k \tau_{ik} = 0$ gives

$$\log \tau_{ik} = \log \pi_k + \sum_{j,\ell} \tau_{j\ell} \log A_{ijk\ell} + \text{cst} \qquad \Leftrightarrow \qquad \tau_{ik} \propto \pi_k \prod_{j,\ell} (A_{ijk\ell})^{\tau_{j\ell}}$$

M step Setting the derivative wrt to each parameter gives

$$\widehat{\pi}_{ik} = \sum_{i} \tau_{ik} / n , \qquad \widehat{\gamma}_{k\ell} = \sum_{i < j} \sum_{k,\ell} \tau_{ik} \tau_{j\ell} \eta_{ij}^{k\ell} / \sum_{i < j} \sum_{k,\ell} \tau_{ik} \tau_{j\ell} .$$

Furthermore, if $f(\cdot, \psi_u) = \mathcal{N}(\cdot, \mu_u, \sigma_u^2)$ (i.e $\psi_u = (\mu_u, \sigma_u^2)$),

$$\hat{\mu}_0 = \sum_{i < j} (1 - \overline{\eta}_{ij}) S_{ij} / \sum_{i < j} (1 - \overline{\eta}_{ij})$$

$$\hat{\sigma}_0^2 = \sum_{i < j} (1 - \overline{\eta}_{ij}) (S_{ij} - \hat{\mu}_0)^2 / \sum_{i < j} (1 - \overline{\eta}_{ij})$$

$$\hat{\mu}_1 = \sum_{i < j} \overline{\eta}_{ij} S_{ij} / \sum_{i < j} \overline{\eta}_{ij} S_{ij}$$

$$\hat{\sigma}_1^2 = \sum_{i < j} \overline{\eta}_{ij} (S_{ij} - \hat{\mu}_0)^2 / \sum_{i < j} \overline{\eta}_{ij} S_{ij}$$

The case of non-parametric version of f_0 and f_1 is considered in Apprendix A.1

By-product The conditional probability for an edge to be part of G is denoted ψ_{ij}^1 :

$$\psi_{ij}^1 := \widetilde{P}\{G_{ij} = 1\} = \sum_{k \mid \ell} \tau_{ik} \tau_{j\ell} \eta_{ij}^{k\ell}$$

and we denote $\psi_{ij}^0 = 1 - \psi_{ij}^1$.

4 Identifiability

4.1 Review of the literature

Notes on identifiability based on papers:

- [1]: "Allman, Elizabeth S. and Matias, Catherine and Rhodes, John A.": Identifiability of parameters in latent structure models with many observed variables
- [2] "Allman, Elizabeth S. and Matias, Catherine and Rhodes, John A.": Parameter identifiability in a class of random graph mixture models
- [5]"Teicher, Henry": Identifiability of Finite Mixtures
- [6] "Teicher, Henry": Identifiability of Mixtures of product measures

What is done in [2] : identifiability in weighted SBM

$$S_{ij}|Z_i = k, Z_j = \ell \sim \mu_{k\ell}$$

$$\mu_{k\ell} = (1 - \gamma_{k\ell})\delta_{\{0\}} + \gamma_{kl}F_{k\ell}(\cdot)$$

for uni dimensional S and symmetric with

- $F_{k\ell}(\cdot)$ parametric (Theorem 12 of [2]): $F(\cdot;\theta_{k\ell})$ under the following assumptions:
 - [A1] The K(K+1)/2 parameter values $\theta_{k\ell}$ are distinct
 - [A2] The family of measures $\mathcal{M} = \{F(\cdot; \theta) | \theta \in \Theta\}$ is such that
 - [A2 (i)] all elements of \mathcal{M} have no point mass at 0
 - [A2 (ii)] the parameters of finite mixtures of measures of \mathcal{M} are identifiable (up to label switching) i.e.

$$\sum_{m=1}^{M} \alpha_m F(\cdots, \theta_m) = \sum_{m=1}^{M} \alpha'_m F(\cdots, \theta'_m) \Rightarrow \sum_{m=1}^{M} \alpha_m \delta_{\theta_m} = \sum_{m=1}^{M} \alpha'_m \delta_{\theta'_m}$$

In particular: true for Gaussian ([5]) and Laplace.

• $F_{k\ell}(\cdot)$ non-parametric (Theorem 14 of [2]): if the $\mu_{k\ell}$ are linearly independent (to be detailed)

About the demonstrations

- Parametric case It is done from the distribution of a triplet (S_{ij}, S_{ik}, S_{jk}) and using [5]. How to adapt it to our case?
- Nonparametric case: only depends on the linear independancy of the $\mu_{k\ell}$. We have to precise it for our case?

4.2 Proof in the parametric uni-dimensional context

I tried to mimic/extend the proof of [2] but I don't think we are in the same scope.

Distribution of the S_{ij}

$$\mathbb{P}(S_{ij}) = \sum_{q,\ell} \pi_q \pi_\ell [(1 - \gamma_{q\ell}) F_0(S_{ij}) + \gamma_{q\ell} F_1(S_{ij})]$$

$$= \left[1 - \sum_{q,\ell} \pi_\ell \pi_q \gamma_{q,\ell}\right] F_0(S_{ij}) + \left[\sum_{q,\ell} \pi_q \pi_\ell \gamma_{q,\ell}\right] F_1(S_{ij})$$

So assuming that F_0 and F_1 are such that any mixture of those two distributions is identifi-

able, we obtain the identifiability of θ_0 , θ_1 and $\sum_{q,\ell} \pi_\ell \pi_q \gamma_{q,\ell}$. So we have identifiability of $\pi' \gamma \pi$. It seems to me that once we have identified θ_0 and θ_1 we will be able to apply to proof of Clisse & al. [3], which is the one I know better. Which is the thing you said: meaning that once we have identified to high level, we are identifiable just like any binary SBM.

Distribution of the triplet (S_{ij}, S_{ik}, S_{jk})

$$\mathbb{P}(S_{ij}, S_{ik}, S_{jk}) = \sum_{q,\ell,m} \pi_q \pi_\ell \pi_m [(1 - \gamma_{q\ell}) F_0(S_{ij}) + \gamma_{q\ell} F_1(S_{ij})] [(1 - \gamma_{qm}) F_0(S_{ik}) + \gamma_{qm} F_1(S_{ik})] \\
= (1 - \gamma_{\ell m}) F_0(S_{jk}) + \gamma_{\ell m} F_1(S_{jk})] \\
= \sum_{q,\ell,m} \sum_{(u,v,w) \in \{0,1\}^3} \eta_{q,\ell,m,u,v} F_u(S_{ij}) F_v(S_{ik}) F_w(S_{jk}) \\
= \sum_{(u,v,w) \in \{0,1\}^3} \left(\sum_{q,\ell,m} \eta_{q,\ell,m,u,v} \right) F_u(S_{ij}) F_v(S_{ik}) F_w(S_{jk}) \\
= \sum_{(u,v,w) \in \{0,1\}^3} \left(\sum_{q,\ell,m} \eta_{q,\ell,m,u,v} \right) F_{u,v,w}(S_{ij}, S_{ik}, S_{jk})$$

with

$$\eta_{q,\ell,m,u,v} = \pi_q \pi_\ell \pi_m (1 - \gamma_{q\ell})^{1-u} \gamma_{q\ell}^u (1 - \gamma_{q\ell})^{1-u} \gamma_{q\ell}^u (1 - \gamma_{qm})^{1-v} \gamma_{qm}^v (1 - \gamma_{\ell m})^{1-w} \gamma_{\ell m}^w$$

The distribution of (S_{ij}, S_{ik}, S_{jk}) is a mixture (weights $= \sum_{q,\ell,m} \eta_{q,\ell,m,u,v}$) of the following distributions

$$F(s) = F_u(s_1, \theta_u) F_v(s_1, \theta_v) F_w(s_1, \theta_w)$$

where $F \in \mathcal{F}$ with

$$\mathcal{F} = \{ F(s; \theta_0, \theta_1) : F(s; \theta_0, \theta_1) = F_u(s_1, \theta_u), F_v(s_2, \theta_v) F_w(s_3, \theta_w), (u, v, w) \in \{0, 1\}^3, \theta_0, \in \Theta_0, \theta_1 \in \Theta_1 \}$$

Assumptions; [A1] we assume that any mixtures of elements of \mathcal{F} is identifiable. (to develop to get assumptions on F_0 and F_1).

The, under assumption [A1], we have:

Then using Theorem 1 of [6] we have the identifiability of any mixture of the product measures.

4.3 Notes from the 20/11/19

Preliminary remarks. Let $nSBM(\pi, \gamma, F_0, F_1)$ denote the noisy SBM model and $SBM(\pi, \alpha)$ the standard binary SBM. [3] showed that $SBM(\pi,\alpha)$ is identifiable provided that all $\overline{\alpha}_k = \sum_{\ell} \pi_{\ell} \alpha_{k\ell}$ are different.

Lemma 1. Let $S \sim nSBM(\pi, \gamma, F_0, F_1)$ and define $B_{ij} = \mathbb{I}\{S_{ij} \leq t\}$. We have that

$$B(t) := [B_{ij}(t)] \sim SBM(\pi, \alpha(t))$$

where, denoting $\Delta(t) = F_1(t) - F_0(t)$,

$$\alpha_{k\ell}(t) = \gamma_{k\ell} F_1(t) + (1 - \gamma_{k\ell}) F_0(t) = F_0(t) + \gamma_{k\ell} \Delta(t).$$

Lemma 2. If the model $SBM(\pi, \gamma)$ is identifiable then the model $SBM(\pi, \alpha(t))$ is identifiable as soon as $\Delta F(t) \neq 0$.

The proof follows: the identifiability of $SBM(\pi, \gamma)$ means that all $\overline{\gamma}_k = \sum_{\ell} \pi_{\ell} \gamma_{k\ell}$ are different, so because all

$$\overline{\alpha}_k(t) = \sum_{\ell} \pi_{\ell} \alpha_{k\ell}(t) = F_0(t) + \overline{\gamma}_k \Delta F(t)$$

are different as soon as $\Delta F(t) \neq 0$.

Parametric case Suppose that F_0 and F_1 belong to a same parametric family, the mixture of which are identifiable. If $S \sim nSBM(\pi, \gamma, F_0, F_1)$, then the marginal distribution is the mixture

$$S_{ij} \sim \overline{\overline{\gamma}} F_1 + (1 - \overline{\overline{\gamma}}) F_0,$$

which is identifiable so $\overline{\overline{\gamma}}$, F_0 and F_1 are identifiable.

Assuming that $SBM(\pi, \gamma)$ is identifiable, we use Lemma 2, picking a threshold t such that $F_0(t) \neq F_1(t)$, to prove the identifiability of π and $\alpha(t)$. A VERIFIER: γ can then be retrieved by solving the K(K+1)/2 equations relating each $\gamma_{k\ell}$ with each $\alpha_{k\ell}(t)$.

Non-parametric case Our aim is to show that if $nSBM(\pi, \gamma, F_0, F_1)$ and $nSBM(\pi', \gamma', F_0', F_1')$ yields the same distribution, then necessarily, $\pi = \pi'$, $\gamma = \gamma'$, $F_0 = F_0'$, $F_1 = F_1'$. We assume that $F_1 > F_0$, so that $\Delta(t) \neq 0$ for all t. If we further assume that $SBM(\pi, \gamma)$ is identifiable, Lemma 2 ensures the identifiability of $SBM(\pi, \alpha(t))$ for all t.

So assume that, any $t \in \mathbb{R}$, $\alpha(t) = \alpha'(t)$, then,

$$\begin{array}{rcl} & (1-\gamma_{k\ell})F_0(t)+\gamma_{k\ell}F_1(t) &=& (1-\gamma_{k\ell}')F_0'(t)+\gamma_{k\ell}'F_1'(t)\\ \Leftrightarrow & F_0(t)+\gamma_{k\ell}\Delta(t) &=& F_0'(t)+\gamma_{k\ell}'\Delta'(t)\\ \text{where} & \Delta(t) &=& F_1(t)-F_0(t) \end{array}$$

This equality is true for any (k, ℓ, t) .

As a consequence

$$\begin{array}{ll} \gamma_{k\ell} & = & \frac{F_0'(t) - F_0(t)}{\Delta(t)} + \gamma_{k\ell}' \frac{\Delta'(t)}{\Delta(t)} \\ & = & A(t) + \gamma_{k\ell}' B(t), \quad \forall t \in \mathbb{R} \end{array}$$

(we used the fact that $\forall t \in \mathbb{R}, \, \Delta(t) = F_1(t) - F_0(t) \neq 0.$)

Let us consider two pairs (k, ℓ) and (k', ℓ') , we have

$$\gamma_{k\ell} = A(t) + \gamma'_{k\ell}B(t)$$

$$\gamma_{k'\ell'} = A(t) + \gamma'_{k'\ell'}B(t)$$

So, if $\gamma'_{k\ell} \neq \gamma'_{k'\ell'}$

$$B(t) = \frac{\gamma_{k\ell} - \gamma_{k'\ell'}}{\gamma'_{k\ell} - \gamma'_{k'\ell'}}$$

So B(t) is a constant function: $B(t)=\frac{\Delta'(t)}{\Delta(t)}=\frac{F_1(t)-F_0(t)}{F_1'(t)-F_0'(t)}=B$ and B>0 Hence

$$F_1(t) - F_0(t) = B(F_1'(t) - F_0'(t))$$

So

$$F_0(t) = F_1(t) - BF_1'(t) + BF_0'(t)$$

Since $t \mapsto B(t)$ is constant then $t \mapsto A(t)$ is also a constant. So

$$A(t) = \frac{F_0'(t) - F_0(t)}{\Delta(t)} = A$$

so

$$F'_0(t) = F_0(t) + A(F_1(t) - F_0(t))$$

$$F'_0(t) = (1 - A)F_0(t) + AF_1(t)$$

$$F_0(t) = \frac{1}{1 - A}F'_0(t) - \frac{A}{1 - A}F_1(t)$$

$$F_0(t) = BF'_0(t) + F_1(t) - BF'_1(t)$$

As a consequence,

$$\frac{1}{1-A}F_0'(t) - \frac{A}{1-A}F_1(t) - BF_0'(t) - F_1(t) + BF_1'(t) = 0$$

$$\frac{1}{1-A}F_0'(t) - \left(1 + \frac{A}{1-A}\right)F_1(t) - BF_0'(t) + BF_1'(t) = 0$$

$$\frac{1}{1-A}F_0'(t) - \frac{1}{1-A}F_1(t) - BF_0'(t) + BF_1'(t) = 0$$

So

$$F_{1}(t) = (1 - B(1 - A))F'_{0}(t) + B(1 - A)F'_{1}(t)$$

$$F_{0}(t) = BF'_{0}(t) + (1 - B(1 - A))F'_{0}(t) + B(1 - A)F'_{1}(t) - BF'_{1}(t)$$

$$= (1 - B(1 - A) + B)F'_{0}(t) - ABF'_{1}(t)$$

$$= (1 + AB)F'_{0}(t) - ABF'_{1}(t)$$

A FINIR: il va falloir jouer sur le support des F_1 et F_0 . Par exemple si on suppose que $F_0(t) = F_0'(t) = 0$ pour un certain t (donc support de F_0 born infrieurement) Alors $ABF_1'(t) = 0$ pour ces t mais $F_1(t) > F_0(t) = 0$ donc A = 0 ou B = 0. Mais B > 0 donc A = 0 donc $F_0'(t) = F_0(t)$. Donc $F_1(t) = F_1'(t)$ et on a fini....

Mais c'est fort comme hypothse. Et surtout a me parat contre intuitif?????

On peut peut-tre seulement mettre des vitesses sur les queues de distributions et travailler en limite?

5 Simulation study

5.1 Simulation design

Data simulation.

- p = 20, 30, 50, 80 nodes
- n = 20, 50, 100, 200 replicates
- K = 3 clusters
- $\pi = (1/6; 1/3, 1/2)$
- γ higher for smaller clusters, density $\overline{\gamma} = \pi^\intercal \gamma \pi = 1.5 \log(p)/p$
- $G \sim SBM(p, \pi, \gamma)$ conditional on G connected
- $\Omega = \text{Laplacian}(G)$ (+ increases the diagonal until positive-definite)
- $(Y_i)_{i=1...n}$ iid $\sim \mathcal{N}(0, \Omega^{-1})$

Inference methods.

oracle: SBM fit on (unobserved) ${\cal G}$

vemGlasso: proposed VEM on glasso scores

vemMB: proposed VEM on M-B scores

vemTree: proposed VEM on tree-based edge probalities

sbmGlasso: pipe-line = SBM on \hat{G}_{glasso} (with eBIC selection)

vemMB: pipe-line = SBM on \hat{G}_{MB} (with ric selection)

vemTree: pipe-line = SBM on \hat{G}_{Tree} (with edge proba > 2/p selection)

6 Illustrations

References

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A Appendix

A.1 Non-parametric emission distributions

Non-parametric estimates. Given a kernel function κ (s.t. $\int \kappa(x) dx = 1$), we propose to estimate the conditional score pdf f_u (u = 0, 1) as

$$\hat{f}_u(s) = \sum_{a < b} w_{ab}^u \kappa(s - S_{ab}), \quad \text{with } \sum_{a < b} w_{ab}^u = 1.$$

For each u=0,1, the maximisation of the lower bound (2) wrt $w^u=(w^u_{ab})_{a< b}$ is equivalent to the maximization of

$$\sum_{i < j} h_{ij}^u \log \hat{f}_u(S_{ij}) - \lambda^u \sum_{a < b} w_{ab}^u$$

with $h^1_{ij} = \sum_{k,\ell} \tau_{ik} \tau_{j\ell} \eta^{k\ell}_{ij}$ and $h^0_{ij} = \sum_{k,\ell} \tau_{ik} \tau_{j\ell} (1 - \eta^{k\ell}_{ij})$. The derivative wrt w^u_{ab} is zero when

$$\sum_{i < j} h_{ij}^u \frac{\kappa(S_{ij} - S_{ab})}{\hat{f}_u(S_{ij})} - \lambda^u = 0,$$

which has no close form solution. However, close-form updates that increase the log-likelihood are provided in Propr. 3 of [4]. We may check if they still hold for the VEM lower bound.

Alternatively, a pragmatic, unjustified choice is to simply set $w_{ab}^u = \psi_{ab}^u$, that is to let each pair (a, b) contribute to the estimation f_1 (resp. f_0) proportionally to the probability for the edge G_{ab} to be equal to 1 (resp. 0).