

# SBM for reconstructed network

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# 1 Introduction

## 2 Model

### Data

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

### Parameters

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

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

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  $G$  :

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

- Distribution of  $G_{ij}$

$$P(G_{ij} = 1 \mid S_{ij}, Z_i = k, Z_j = \ell) = \frac{\gamma_{k\ell} f_1(S_{ij})}{\gamma_{k\ell} f_1(S_{ij}) + (1 - \gamma_{k\ell}) f_0(S_{ij})} =: \eta_{ij}^{k\ell}$$

$$\tilde{P}(G_{ij} = 1 \mid S_{ij}) = \sum_{k, \ell} \tau_{ik} \tau_{j\ell} \eta_{ij}^{k\ell} =: \bar{\eta}_{ij}$$

- Kullback-Leibler divergence

$$KL(q(U); p(U)) = \mathbb{E}_q(\log q(U) - \log p(U))$$

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

$$= KL(q(U); p(U)) + \mathbb{E}_{q(U)} KL(q(V \mid U), p(V \mid U))$$

### 3 Inference

#### 3.1 Loss function

**Log-likelihood**

$$\begin{aligned}\log p(Z, G, S) &= \log p(Z; \pi) + \log p(G \mid Z; \gamma) + \log p(S \mid G; \psi) \\ &= \sum_{i,k} Z_{ik} \log \pi_k + \sum_{i < j} \sum_{k,\ell} Z_{ik} Z_{j\ell} (G_{ij} \log \gamma_{k\ell} + (1 - G_{ij}) \log(1 - \gamma_{k\ell})) \\ &\quad + \sum_{i < j} G_{ij} \log f_1(S_{ij}) + (1 - G_{ij}) \log f_0(S_{ij})\end{aligned}$$

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

$$q(Z, G) = q(Z)q(G \mid Z) := q(Z)p(G \mid Z, S) \quad (1)$$

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

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

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

**Lower bound**  $J(\theta, q)$

$$\begin{aligned}J(\theta, q) &= \log p_\theta(S) - KL(q(Z, G); p(Z, G \mid S)) \\ &= \mathbb{E}_q \log p_\theta(Z, G, S) + H(q(Z)) + \mathbb{E}_q H(q(G \mid Z))\end{aligned} \quad (2)$$

$$\begin{aligned}&= \sum_{i,k} \tau_{ik} \log \pi_k + \sum_{i < j} (\bar{\eta}_{ij} \log \gamma_{k\ell} + (1 - \bar{\eta}_{ij}) \log(1 - \gamma_{k\ell})) \\ &\quad + \sum_{i < j} \sum_{k,\ell} \tau_{ik} \tau_{j\ell} (\eta_{ij}^{k\ell} \log f_1(S_{ij}) + (1 - \eta_{ij}^{k\ell}) \log f_0(S_{ij})) \\ &\quad - \sum_{i,k} \tau_{ik} \log \tau_{ik} - \sum_{i < j} \sum_{k,\ell} \tau_{ik} \tau_{j\ell} (\eta_{ij}^{k\ell} \log \eta_{ij}^{k\ell} + (1 - \eta_{ij}^{k\ell}) \log(1 - \eta_{ij}^{k\ell}))\end{aligned} \quad (3)$$

#### 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  $\tau_{ik}$  to zero with the constraint  $\sum_k \tau_{ik} = 0$  gives

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

**M step** Setting the derivative wrt to each parameter gives

$$\hat{\pi}_{ik} = \sum_i \tau_{ik} / n , \quad \hat{\gamma}_{k\ell} = \sum_{i < j} \sum_{k, \ell} \tau_{ik} \tau_{j\ell} \eta_{ij}^{k\ell} \Big/ \sum_{i < j} \sum_{k, \ell} \tau_{ik} \tau_{j\ell} .$$

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

$$\begin{aligned} \hat{\mu}_0 &= \sum_{i < j} (1 - \bar{\eta}_{ij}) S_{ij} \Big/ \sum_{i < j} (1 - \bar{\eta}_{ij}) & \hat{\sigma}_0^2 &= \sum_{i < j} (1 - \bar{\eta}_{ij}) (S_{ij} - \hat{\mu}_0)^2 \Big/ \sum_{i < j} (1 - \bar{\eta}_{ij}) \\ \hat{\mu}_1 &= \sum_{i < j} \bar{\eta}_{ij} S_{ij} \Big/ \sum_{i < j} \bar{\eta}_{ij} S_{ij} & \hat{\sigma}_1^2 &= \sum_{i < j} \bar{\eta}_{ij} (S_{ij} - \hat{\mu}_0)^2 \Big/ \sum_{i < j} \bar{\eta}_{ij} S_{ij} \end{aligned}$$

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

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

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

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

$$\begin{aligned} S_{ij}|Z_i = k, Z_j = \ell &\sim \mu_{k\ell} \\ \mu_{k\ell} &= (1 - \gamma_{k\ell})\delta_{\{0\}} + \gamma_{k\ell}F_{k\ell}(\cdot) \end{aligned}$$

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.

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

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  $S_{ij}$**

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

So assuming that  $F_0$  and  $F_1$  are such that any mixture of those two distributions is identifiable, we obtain the identifiability of  $\theta_0, \theta_1$  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  $\theta_0$  and  $\theta_1$  we will be able to apply to proof of Céliste & 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 $(S_{ij}, S_{ik}, S_{jk})$

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

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

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

**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  $\bar{\alpha}_k = \sum_\ell \pi_\ell \alpha_{k\ell}$  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  $\bar{\gamma}_k = \sum_\ell \pi_\ell \gamma_{k\ell}$  are different, so because all

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

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

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

which is identifiable so  $\bar{\gamma}$ ,  $F_0$  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  $\pi$  and  $\alpha(t)$ . **A VERIFIER :**  $\gamma$  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,

$$\begin{aligned} (1 - \gamma_{k\ell})F_0(t) + \gamma_{k\ell}F_1(t) &= (1 - \gamma'_{k\ell})F'_0(t) + \gamma'_{k\ell}F'_1(t) \\ \Leftrightarrow F_0(t) + \gamma_{k\ell}\Delta(t) &= F'_0(t) + \gamma'_{k\ell}\Delta'(t) \\ \text{where } \Delta(t) &= F_1(t) - F_0(t) \end{aligned}$$

This equality is true for any  $(k, \ell, t)$ .

As a consequence

$$\begin{aligned} \gamma_{k\ell} &= \frac{F'_0(t) - F_0(t)}{\Delta(t)} + \gamma'_{k\ell} \frac{\Delta'(t)}{\Delta(t)} \\ &= A(t) + \gamma'_{k\ell}B(t), \quad \forall t \in \mathbb{R} \end{aligned}$$

(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  $(k, \ell)$  and  $(k', \ell')$ , we have

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

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  $B > 0$ .

Moreover we get

$$\gamma_{k\ell} - \gamma_{k'\ell'} = B(\gamma'_{k\ell} - \gamma'_{k'\ell'}), \quad \forall (k, \ell, k', \ell').$$

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

$$\begin{aligned} F'_0(t) &= F_0(t) + A(F_1(t) - F_0(t)) \\ F'_0(t) &= (1 - A)F_0(t) + AF_1(t) \\ F_0(t) &= \frac{1}{1 - A}F'_0(t) - \frac{A}{1 - A}F_1(t) \\ F_0(t) &= BF'_0(t) + F_1(t) - BF'_1(t) \end{aligned}$$

As a consequence,

$$\begin{aligned} \frac{1}{1 - A}F'_0(t) - \frac{A}{1 - A}F_1(t) - BF'_0(t) - F_1(t) + BF'_1(t) &= 0 \\ \frac{1}{1 - A}F'_0(t) - \left(1 + \frac{A}{1 - A}\right)F_1(t) - BF'_0(t) + BF'_1(t) &= 0 \\ \frac{1}{1 - A}F'_0(t) - \frac{1}{1 - A}F_1(t) - BF'_0(t) + BF'_1(t) &= 0 \end{aligned}$$



So

$$\begin{aligned}
F_1(t) &= (1 - B(1 - A))F'_0(t) + B(1 - A)F'_1(t) \\
F_0(t) &= BF'_0(t) + (1 - B(1 - A))F'_0(t) + B(1 - A)F'_1(t) - BF'_1(t) \\
&= (1 - B(1 - A) + B)F'_0(t) - ABF'_1(t) \\
&= (1 + AB)F'_0(t) - ABF'_1(t) \\
&= F'_0(t) - AB(F'_1(t) - F'_0(t)) \\
F_0(t) - F'_0(t) &= AB(F'_0(t) - F'_1(t))
\end{aligned}$$

**A FINIR** : il va falloir jouer sur le support des  $F_1$  et  $F_0$ .

On a  $F_1(t) < F_0(t)$  si on veut que en moyenne les valeurs sous  $F_1$  soient plus grandes que celles sous  $F_0$ .

Si il existe  $\tau$  tel que  $F_0(\tau) = 1 = F'_0(\tau)$  alors en ce point,  $1 = 1 - AB(F'_1(\tau) - F'_0(\tau))$  donc  $AB(F'_1(\tau) - 1)$ ; Or  $F'_1(\tau) < F'_0(\tau)$  donc  $AB = 0$ . Or  $B > 0$  donc  $A = 0$  Donc  $F'_0(t) = F_0(t)$ .

On peut peut-être 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
- $\pi = (1/6; 1/3, 1/2)$
- $\gamma$  higher for smaller clusters, density  $\bar{\gamma} = \pi^\top \gamma \pi = 1.5 \log(p)/p$
- $G \sim SBM(p, \pi, \gamma)$  conditional on  $G$  connected
- $\Omega = \text{Laplacian}(G)$  (+ increases the diagonal until positive-definite)
- $(Y_i)_{i=1\dots n}$  iid  $\sim \mathcal{N}(0, \Omega^{-1})$

#### Inference methods.

**oracle** : SBM fit on (unobserved)  $G$

**vemGlasso** : proposed VEM on glasso scores

**vemMB** : proposed VEM on M-B scores

**vemTree** : proposed VEM on tree-based edge probabilities

**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

### Références

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## A Appendix

### A.1 Non-parametric emission distributions

**Non-parametric estimates.** Given a kernel function  $\kappa$  (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  $w^u = (w_{ab}^u)_{a < b}$  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  $h_{ij}^1 = \sum_{k, \ell} \tau_{ik} \tau_{j\ell} \eta_{ij}^{k\ell}$  and  $h_{ij}^0 = \sum_{k, \ell} \tau_{ik} \tau_{j\ell} (1 - \eta_{ij}^{k\ell})$ . The derivative wrt  $w_{ab}^u$  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).