Mixture tree model for network inference

JOBIM

Raphaëlle Momal

UMR518 AgroParis Tech/INRA

June 21, 2018

1 Motivation

2 Network inference
- General Framework
- Using trees

3 With count data
- Model
- Illustration

Context

Rising interest in jointly analysed species abundances:

- Metagenomics
- Microbiologie
- Ecology

Ecological network

Tool to better understand species interactions (direct/indirect, nature), eco-systems organizations (clusters ?)

Allows for resilience analyses, pathogens control, ecosystem comparison, reaction prediction...

Example

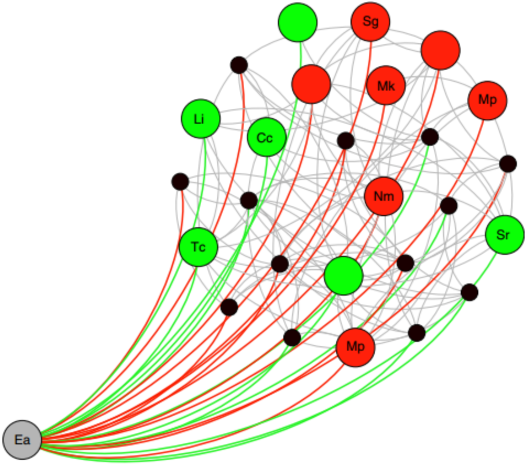


Figure: *Erysiphe alphitoides* pathobiom on oak tree leaves.

Data

- Species : animal, bacteria, gene ...
- Abundances : ecological counts, Next-Generation Sequencing technologies...
- Covariates : coverage, temperature, water depth ...

Repeated signal : n samples of p abundances.

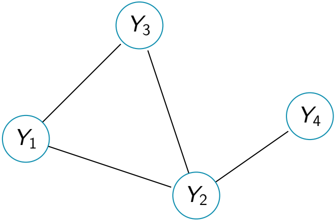
Notations

$Y = [Y_{ij}]_{(i,j)\in\{1,\dots,n\}\times\{1,\dots,p\}}$

- Y_{ij} : abundance of the j^{th} species in the i^{th} sample

Infer the species interaction network from Y

Graphical models



- All variables are dependant
- Some are conditionnally independant (i.e. indirectly dependant)

$$Y_4 \perp\!\!\!\perp (Y_1, Y_3) | Y_2$$

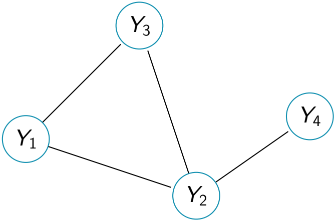
Graphical models

Factorization propriety

The joint distribution P is faithful to the graph G iff

$$P(Y_1, \dots, Y_p) \propto \prod_{C \in \mathcal{C}_G} \psi_C(Y_C)$$

where $\mathcal{C}_G$ = set of cliques of G.



$$P(Y_1, Y_2, Y_3, Y_4) \propto \psi_1(Y_1, Y_2, Y_3) \times \psi_2(Y_3, Y_4)$$

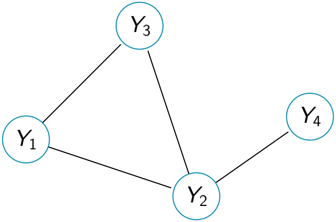
Gaussian Graphical Models (GGM)

Gaussian distribution.

$$Y_r \sim \mathcal{N}_p(\mu, \Sigma)$$

μ = vector of means, Σ = covariance matrix.

A nice property.



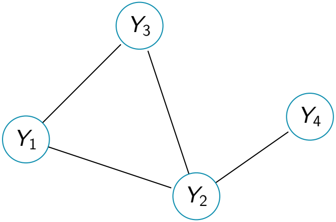
Gaussian Graphical Models (GGM)

Gaussian distribution.

$$Y_r \sim \mathcal{N}_p(\mu, \Sigma)$$

$\mu =$ vector of means, $\Sigma =$ covariance matrix.

A nice property.



Adjacency matrix

$$A = \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

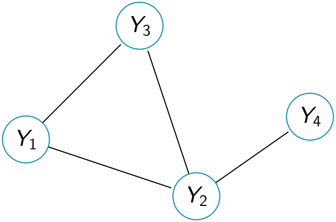
Gaussian Graphical Models (GGM)

Gaussian distribution.

$$Y_r \sim \mathcal{N}_p(\mu, \Sigma)$$

μ = vector of means, Σ = covariance matrix.

A nice property.



Covariance matrix

$$\Sigma \propto \begin{bmatrix} 1 & -.25 & -.41 & .25 \\ -.25 & 1 & -.41 & .25 \\ -.41 & -.41 & 1 & -.61 \\ .25 & .25 & -.61 & 1 \end{bmatrix}$$

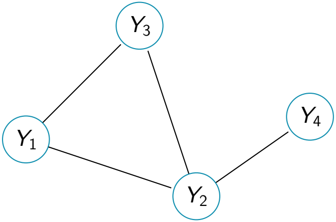
Gaussian Graphical Models (GGM)

Gaussian distribution.

$$Y_r \sim \mathcal{N}_p(\mu, \Sigma)$$

$\mu =$ vector of means, $\Sigma =$ covariance matrix.

A nice property.



Inverse covariance matrix

$$\Sigma^{-1} \propto \begin{bmatrix} 1 & .5 & .5 & 0 \\ .5 & 1 & .5 & 0 \\ .5 & .5 & 1 & .5 \\ 0 & 0 & .5 & 1 \end{bmatrix}$$

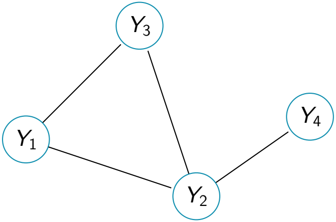
Gaussian Graphical Models (GGM)

Gaussian distribution.

$$Y_r \sim \mathcal{N}_p(\mu, \Sigma)$$

$\mu =$ vector of means, $\Sigma =$ covariance matrix.

A nice property.



Estimated inverse covariance matrix

$$\widehat{\Sigma}^{-1} \propto \begin{bmatrix} 1 & .48 & .61 & .09 \\ .48 & 1 & .67 & .06 \\ .61 & .67 & 1 & .46 \\ .09 & .06 & .46 & 1 \end{bmatrix}$$

$(n = 100)$

Sparse with Glasso

Sparsity assumption $\Rightarrow$ find a sparse estimate for $\Omega = \Sigma^{-1}$

Negative log-likelihood :

$$L(Y,\Omega) \propto \frac{n}{2}\log(det(\Omega)) - \frac{n}{2} Y^T \Omega Y$$

Graphical LASSO (glasso) :

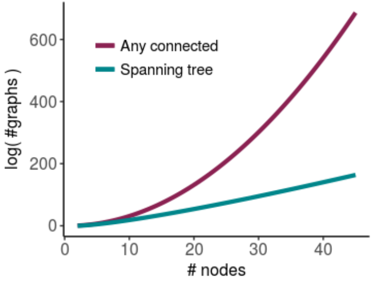
Glasso penalises the L_1 norm of the concentration matrix:

$$\widehat{\Omega}_\lambda = \arg\min_{\Omega \in \mathcal{S}_d^+} \left\{ L(Y,\Omega) + \lambda \sum_{i \neq j} |w_{ij}| \right\}$$

Spanning trees

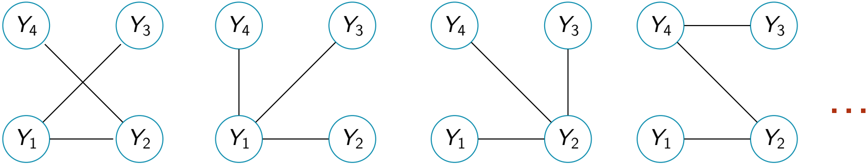
Spanning trees are another sparse solution :

$$\left.\begin{array}{l} G \text{ is connected} \\ G \text{ has no cycle} \end{array}\right\} G \text{ has } (p-1) \text{ edges}$$



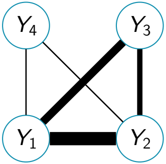
Much smaller space to explore:
$\#\mathcal{G} = 2^{\frac{p(p-1)}{2}}$ vs. $\#\mathcal{T} = p^{(p-2)}$

Tree averaging



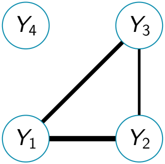
$P\{T = T_1 | Y\}$ $P\{T = T_2 | Y\}$ $P\{T = T_3 | Y\}$ $P\{T = T_4 | Y\}$

Compute edge probabilities:



$P\{(j, k) \in T | Y\}$

Thresholding probabilities:



$P\{(j, k) \in T | Y\}$

PLN model

Poisson log-Normal distribution

$$\left.\begin{array}{ll} Z_i \ iid & \sim \mathcal{N}_d(\mu, \Sigma) \\ & (Y_{ij})_j \perp\!\!\!\perp |Z_i \\ Y_{ij}|Z_{ij} & \sim \mathcal{P}(e^{Z_{ij}}) \end{array}\right\} Y \sim \mathcal{PLN}(\mu, \Sigma)$$

- Gaussian latent layer
- Easily generalized to multi-variate data (contrary to Negative binomial distribution)

PLN model

Poisson log-Normal distribution

$$\left.\begin{array}{ll} Z_i \ iid & \sim \mathcal{N}_d(\mu, \Sigma) \\ & (Y_{ij})_j \perp\!\!\!\perp | Z_i \\ Y_{ij}|Z_{ij} & \sim \mathcal{P}(e^{x_i^{\intercal}\Theta_j + Z_{ij}}) \end{array}\right\} Y \sim \mathcal{PLN}(x^{\intercal}\Theta + \mu, \Sigma)$$

- Gaussian latent layer
- Easily generalized to multi-variate data (contrary to Negative binomial distribution)
- Allow adjustment for covariates

PLN model

Poisson log-Normal distribution

$$\left.\begin{array}{ll} Z_i \ iid & \sim \mathcal{N}_d(\mu, \Sigma) \\ & (Y_{ij})_j \perp\!\!\!\perp |Z_i \\ Y_{ij}|Z_{ij} & \sim \mathcal{P}(e^{x_i^\intercal \Theta_j + Z_{ij}}) \end{array}\right\} Y \sim \mathcal{PLN}(x^\intercal \Theta + \mu, \Sigma)$$

- Gaussian latent layer
- Easily generalized to multi-variate data (contrary to Negative binomial distribution)

Idea: Infer the latent Gaussian network.

Oak Mildew