

Lab 6 - Advanced Machine Learning

Probabilistic graph model

Pierre HOUDOUIN

CentraleSupélec

03 Novembre 2023



CentraleSupélec

General information

- **Assignment** : Alone or in pairs, you will code the algorithms you learnt in Scikit-learn formalism'
- **Due** : Each assignment has to be sent at most 7 days after the lab session at pierre.houdouin@centralesupelec.fr
- **Grading** : There are 5 lab sessions, each lab session is worth 4 points, the average will count for half of your final grade
- **Questions** : If you have questions, comments or feedbacks about the lab session, feel free to contact me by email



Lesson recap

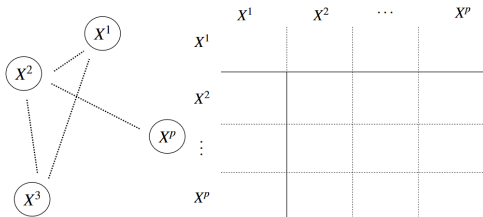
Graphical model

Suppose we have a random vector $X = (X_1, \dots, X_p)$:

no edge between node i and j

$\iff X_i$ and X_j are conditionally independant

$\iff X_i$ and X_j have 0 inverse correlation (gaussian case)



\longrightarrow need to estimate $\Lambda = \Sigma^{-1}$

Estimation of the precision matrix

Classic

Use the Maximum Likelihood :

$$\min_{\Lambda > 0} -\log \det \Lambda + \text{Tr}(S\Lambda) \quad \Rightarrow \quad \hat{\Lambda} = S^{-1} = \left(\frac{1}{n} \sum_{i=1}^n (x_i - \hat{\mu})(x_i - \hat{\mu})^T \right)^{-1} \quad \text{where } \hat{\mu} = \frac{1}{n} \sum_{i=1}^n x_i$$

closed-form inverse empirical covariance empirical mean

not great when $n < p$: reduce #parameters via a sparsity constraint

GLASSO

Use the Sparse Maximum Likelihood :

$$\min_{\Lambda > 0} -\log \det \Lambda + \text{Tr}(S\Lambda) + \lambda \|\Lambda\|_1 \quad \Rightarrow \quad T_k \leftarrow Y_{k-1} - Z_{k-1} - \frac{S}{\nu} \quad \begin{array}{l} \text{intermediate step for computations} \\ \nu > 0 \text{ weight of the penalization } Y = \Lambda \end{array}$$

reformulate \downarrow ADMM algo

$$\Lambda_k \leftarrow \frac{1}{2} \text{diag} \left(\left\{ \lambda_i(T_k) + \sqrt{\lambda_i(T_k)^2 + \frac{4}{\nu}} \right\} \right) \quad \text{primal variable}$$

$$Y_k \leftarrow \text{ST}_{(\lambda/\nu)}(\Lambda_k + Z_{k-1}) \quad \text{relaxed primal variable}$$

$$Z_k \leftarrow Z_{k-1} + \nu (\Lambda_k - Y_k) \quad \text{dual variable}$$



Estimation of the precision matrix

Nodewise regression

Learn the support of the precision matrix via sparse linear regressions :

predict each variable X^j using the others $\{X^k, k \neq j\}$ with LASSO $\rightarrow \beta^j \in \mathbb{R}^{p-1}$ weights of the regression...

then deduce the support : $\Lambda_{jk} \neq 0 \iff \hat{\beta}_k^j \text{ AND } \hat{\beta}_j^k \text{ are non-zero}$...used as edge-activators
(also try OR)



Assignment plan

- **Part 1** : Implement your own Graphical LASSO
- **Part 2** : Implement your own Node-wise Regression algorithm
- **Part 3** : Application to simulated data

