Objective Bayesian model selection in general Gaussian graphical models

Mathilde Bouriga

EDF R&D Département OSIRIS - Université Paris-Dauphine

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Application context

Market-risk assessment for high-dimensional asset portfolio.

- Portfolio variation $V_{t,t+h}$ between $t$ and $t+h$ affected by risk factors, specifically by price returns $X$ of portfolio products.

- A widely used risk measure: Value-at-risk. $\text{VaR}_{1-\alpha}$ at a risk level $\alpha$ over a given time horizon $h$ = the $\alpha$-quantile of the portfolio variation between $t$ and $t+h$.

$$Pr(V_{t,t+h} < \text{VaR}_{1-\alpha}) = \alpha\%.$$
VaR Computation

- Method = the analytic VaR, built on 2 assumptions:
  1. portfolio variation as a linear combination of product returns, \( V_{t,t+h} = a^T X_{t,t+h} \),
  2. normal distribution assumptions about returns, \( X_{t,t+1} | \Sigma \sim \mathcal{N}_p(0, \Sigma) \).

\[ \Rightarrow \text{VaR}_{1-\alpha} = \sqrt{h} \sqrt{a^T \hat{\Sigma} a} \Phi^{-1}(\alpha) \], calculated from \( \hat{\Sigma} \), with \( \Phi^{-1}(\alpha) \) the \( \alpha \)-quantile of the standard normal distribution.

- Problem: sensitivity of VaR results to variations of \( \hat{\Sigma} \) + unstable matrix estimator, as with a small sample.

\[ \leftarrow \text{Requirement: stable covariance matrix between returns.} \]
Data

- Portfolio made of 27 energy products.
- The covariance matrix for the returns $X$ on the products in the portfolio to estimate, *i.e* 378 elements to estimate.
- Matrix to estimate from 200 observations.
Problem formalization

$$X|\Sigma \sim \mathcal{N}_p(0, \Sigma),$$

where $\Sigma$ is a $p \times p$ symmetric positive-definite matrix.

Problem: **Estimation of** $\Sigma$ from a sample of $X$, $X=(X_1, \ldots, X_n)$ where $p$ is close to $n$.

Classical estimator based on the scatter matrix $S_n = X^TX$:

- unstable estimator
- distortion of the eigenstructure
- $S_n$ no longer positive definite if $p \geq n.$
General approaches to induce stability over the unstructured classical estimator of the covariance matrix:

- by shrinking of eigenvalues,
- by shrinking this estimate toward a parsimonious, structured form of the matrix,
- by imposing various restrictions on the model and then estimating covariance matrix related to these structural assumptions.
Alternatives

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Bayesian inference on covariance matrices in Gaussian Graphical models

⇒ Visual aid - interpretation / Aid in parameter estimation
Graph theory

An undirected graph is a pair $G = (V, E)$ with vertex set $V$ and edge set $E = \{(i, j)\}$ for some pairs $(i, j) \in V$.

A clique $C$ of $G$ is a set of pairwise adjacent vertices.

Figure: Graph $G$ with 5 nodes and 6 edges.
Matrix theory

Let $\Sigma$ be a matrix, the *G*-incomplete symmetric matrix $\Sigma^E$ is defined as an incomplete symmetric matrix indexed by $V \times V$, in which the elements are those of $\Sigma_{ij}$ for all $(i,j) \in E$, and with the remaining elements unspecified.

$$
\Sigma^E = \begin{pmatrix}
\sigma_{11} & \sigma_{12} & * & * & \sigma_{15} \\
\sigma_{21} & \sigma_{22} & \sigma_{23} & \sigma_{14} & * \\
* & \sigma_{32} & \sigma_{33} & \sigma_{34} & * \\
* & \sigma_{42} & \sigma_{43} & \sigma_{44} & \sigma_{45} \\
\sigma_{51} & * & * & \sigma_{54} & \sigma_{55}
\end{pmatrix}
$$

A *completion* of an incomplete matrix is a specific choice of values for the unspecified entries.
Gaussian graphical model GGM (1)

A GGM uses a graphical structure to define a set of pairwise conditional independence relationships.

- With precision matrix \( \Omega = \Sigma^{-1} \), \( X_i \) and \( X_j \) of \( X \) are conditionally independent (given the neighboring variables of each) iff \( \omega_{ij} = 0 \).

- If \( G = (V, E) \) is an undirected graph whose vertices are associated with \( X \), \((|V| = p)\), \( \omega_{ij} = 0 \) for all pairs \((i, j) \notin E\).

\[
\begin{pmatrix}
\omega_{11} & \omega_{12} & 0 & 0 & \omega_{15} \\
\omega_{21} & \omega_{22} & \omega_{23} & \omega_{14} & 0 \\
0 & \omega_{32} & \omega_{33} & \omega_{34} & 0 \\
0 & \omega_{42} & \omega_{43} & \omega_{44} & \omega_{45} \\
\omega_{51} & 0 & 0 & \omega_{54} & \omega_{55}
\end{pmatrix}
\iff X_1 \perp X_3 | X_2, X_4, X_5 \ldots
\]
Let $G = (V, E)$ and $M^+(G)$ denote the cone of $|V| \times |V|$ positive definite matrices such that $ij$ entry is equal to 0 whenever $(i, j) \notin E$.

A GGM with graph $G$ is

$$\mathcal{M}_G = \{ \mathcal{N}(0, \Sigma) | \Omega = \Sigma^{-1} \text{ and } \Omega \in M^+(G) \}.$$ 

On the covariance space, incomplete matrices $\Sigma^E$ to handle: far from simple.
Two challenging problems for covariance estimation in GGM

1. graphical model selection problem
   = problem of estimating the zero-pattern of $\Omega$,

2. covariance matrix estimation based on the model selected.
Two challenging problems for covariance estimation in GGM

1. Graphical model selection problem
   = problem of estimating the zero-pattern of $\Omega$,

2. Covariance matrix estimation based on the model selected.
   
   in a Bayesian framework.

\[ X|\Sigma \sim \mathcal{N}_p(0, \Sigma), \quad \Omega = \Sigma^{-1} \in M^+(G) \]

Parameters: $\Omega$, nuisance parameter, and $G$, parameter of interest.

- Priors to handle: $\pi(\Omega, G) = \pi(\Omega|G)\pi(G)$,
- Posterior to handle: $\pi(G|X) = \int \pi(\Omega, G|X) d\Omega$,
- Estimator to choose: $\hat{G}$. 
With our real data

Example: focus on the 9 first variables. Starting from the empirical covariance matrix, we seek to reduce problem complexity and find the underlying conditional-dependency structures.

$$\begin{bmatrix}
1.00 & 0.85 & 0.76 & 0.75 & 0.64 & 0.72 & 0.66 & 0.58 & 0.60 \\
0.85 & 1.00 & 0.94 & 0.79 & 0.72 & 0.74 & 0.70 & 0.63 & 0.62 \\
0.76 & 0.94 & 1.00 & 0.88 & 0.78 & 0.75 & 0.73 & 0.64 & 0.66 \\
0.75 & 0.79 & 0.88 & 1.00 & 0.80 & 0.76 & 0.67 & 0.70 & 0.62 \\
0.64 & 0.72 & 0.80 & 0.80 & 1.00 & 0.63 & 0.69 & 0.77 & 0.65 \\
0.72 & 0.74 & 0.80 & 0.83 & 1.00 & 0.71 & 0.90 & 0.64 & 0.62 \\
0.86 & 0.89 & 0.73 & 0.76 & 0.69 & 0.71 & 1.00 & 0.60 & 0.98 \\
0.39 & 0.63 & 0.64 & 0.67 & 0.77 & 0.93 & 0.60 & 1.00 & 0.98 \\
0.80 & 0.82 & 0.56 & 0.70 & 0.63 & 0.64 & 0.95 & 0.99 & 1.00
\end{bmatrix}$$

Figure: $$X^TX$$ and the underlying structure.
Substantial problems

• Which priors, $\pi(\Sigma|G)$ and $\pi(G)$, for efficient model search? (explicit expression for prior in the decomposable case)

• Properness conditions for the posterior distribution? (easier to derive in the decomposable case)

• Which tool to model comparison? (depending on the choice of priors: proper or not)

• Which graphical model-selection procedure? (search computationally less expensive in the decomposable case)
Decomposable or non-decomposable graphs?

Decomposition

\((A, B, C)\), subsets of \(V\), form a *decomposition* of \(G\) if \(C\) is complete, *i.e* a set of pairwise adjacent vertices, and \(C\) is separator of \(A, B\), *i.e* any path from \(A\) to \(B\) goes through \(C\).

A sequence of subgraphs that cannot be decomposed further are the *prime components* of a graph; if every prime component is clique, the graph is *decomposable*.

Any given graph can \(G\) be embedded in a decomposable graph by adding edges, the decomposable graph is called a *triangulation* of \(G\).
A = \{X_1, X_2, X_4, X_5\} is a prime component, B = \{X_2, X_3, X_4\} is a clique and \( C = \{X_2, X_4\} \) is a separator.
Figure: Triangulated graph.

All the prime components are cliques.
Although, in the literature, attention is often restricted to the decomposable case, only a small fraction of the total number of graphs on $p$ nodes is decomposable.

**Figure:** Proportion of decomposable graphs depending on the number of vertices.

$\Rightarrow$ Graphical model selection for general graphs.
We choose to consider a Bernoulli distribution on the edge inclusion indicators with success probability $\beta$.

$$\pi(G \text{ with } k \text{ edges}|\beta) \propto \beta^k (1 - \beta)^{m-k}$$

with $m = \frac{p(p-1)}{2}$, the maximum number of possible edges.

$\beta = \frac{1}{p-1}$ will encourage sparse graphs.
Standard prior for $\Omega$ in the literature (1)

As the GGM with graph $G = (V, E)$ is a regular exponential family [Lau96] with canonical parameter $\Omega$, the standard conjugate prior for $\Omega$ in $M^+(G)$ can be written as

$$\pi_G(\Omega | \delta, D^E) = \frac{1}{Z(G, \delta, D^E)}|\Omega|^{(\delta-2)/2} \exp \left\{ - \frac{1}{2} tr(\Omega D^E) \right\}$$

where $\delta, D^E$ are such that the normalizing constant $Z(G, \delta, D^E)$ is finite.
Standard prior for $\Omega$ (2)

\[
\int_{M^+(G)} |\Omega|^{(\delta-2)/2} \exp \left\{ -\frac{1}{2} tr(\Omega D^E) \right\} d\Omega < \infty
\]

if $\delta > 2$ and the incomplete matrix $D^E$ admits a positive completion.

In this case, it is called $\text{G-Wishart}$ distribution with parameters $(\delta, D^E)$.

- In decomposable cases, $Z(G, \delta, D^E)$ available in a closed form,
- in non-decomposable cases, $Z(G, \delta, D^E)$ not available in a closed form.
A new objective prior for $\Omega$ (1)

We propose to consider this noninformative prior for $\Omega$ of a GGM with arbitrary graph $G$:

$$\pi_N(\Omega|G) \propto |\Omega|^{-1} \text{ for } \Omega \in M^+(G).$$

- Choice motivation: the involved default-procedure for GGM selection yields efficient posterior separation of models.
- A particular case: this distribution corresponds to the prior proposed by [CS07] for model selection when considering only the decomposable graphs.
Proposition: The posterior density of $G$

$$
\pi(G|\mathbf{X}) \propto \frac{1}{p-1} \frac{m(p-2)^{m-k}}{\sqrt{2\pi}^{np}} Z(G, n, \mathbf{X}^T\mathbf{X}) \text{ with } m = \frac{p(p-1)}{2}
$$

is proper iff

$$
Z(G, n, (\mathbf{X}^T\mathbf{X})^E) = \int_{M^+(G)} |\Omega|^\frac{n-2}{2} \exp \{-1/2tr(\Omega(\mathbf{X}^T\mathbf{X})^E)\} \, d\Omega
$$

is finite.

Sufficient conditions:

• $n > 2$

• $(\mathbf{X}^T\mathbf{X})^E$ has a positive completion: condition hard to find for general graphs.
Proposition: Let $G^+ = (V, E^+)$ be a minimal triangulation of $G$ - a decomposable graph where $E^+ \supset E$, with the property that removal of any edge in $G^+$ which is not an edge in $G$ will not be decomposable.

Let $C^+$ denote the set of cliques of $G^+$.

$$n > \max_{C \in C^+} |C^+| \Rightarrow (X^T X)^E$$ has a positive completion.

Particular case: for the full graph, well-known condition.

Conclusion:

- $\pi(G|X)$ proper for all the graphs, when $n > p$.
- If $n \leq p$, restriction on the graphs under consideration. $\pi(G|X)$ proper for any graph in $S_G = \{ G | Z(G, n, (X^T X)^E) < \infty \}$. 
Structural learning in Gaussian graphical models usually involves assessing the posterior probability of the graphs to evaluate

$$\frac{\pi(G_1|X)}{\pi(G_2|X)} = \frac{\pi(G_1)}{\pi(G_2)} BF_{12}(X),$$

where

$$BF_{12}(X) = \frac{f(X|G_1)}{f(X|G_2)},$$

where $f(X|G_i) = \int_{M^+(G)} f(X|\Omega_i, G_i) \pi_i(\Omega|G_i) d\Omega_i$ is the marginal likelihood of $G_i$.

Bayesian model comparison is usually based on Bayes factors.
Fractional Bayes factors

**Definition**

Using improper priors for parameters in alternative models ⇒ Bayes factors not well defined:

\[
BF_{12}(X) = \frac{c_1 f(X|G_1)}{c_2 f(X|G_2)}, \quad \text{with } \frac{c_1}{c_2} \text{ unknown.}
\]

Alternative key: Fractional Bayes factors (FBF) introduced by [O’H95] among Partial Bayes factors (PBF) [Per05].

\[
FBF_{12}(X) = \frac{q(X|G_1, g)}{q(X|G_2, g)},
\]

with \( q(X|G, g) = \int_{M^+(G)} f(X|\Omega)^{1-g} \pi_g(\Omega|G, X, g) d\Omega \), the *fractional marginal likelihood* of \( G \).
Graph score based on Laplace approximations

\[ q(X|G, g) = \frac{1}{\sqrt{2\pi}^{np}} \frac{Z(G, n, X^T X)}{Z(G, gn, gX^T X)} \quad \text{for } ng > 2. \]

We use the diagonal Laplace approximation proposed by [LD10] to estimate \( Z(G, ., .) \) for any graph \( G \).
A challenging issue

• $p$ nodes in a graph $\Rightarrow m = \frac{p(p-1)}{2}$ possible edges $\Rightarrow 2^m$ possible graphs.
  Beyond $p = 7$, enumeration becomes a practical impossibility.

• Need to scalable search methodologies that are capable of finding good models, or at least distinguishing the important edges from the irrelevant ones.

• Main classes of graphical model-selection procedures: compositional methods and direct search.

$\implies$ Framework proposed by [BMM09] which is a direct search method initialized with a set of graphs issued from a compositional method.
An heuristic search technique

An iterative algorithm which tries to identify the most likely graphs, inspired by [SC08].

At time $t$, starting with

- $t - 1$ distinct explored graphs ($G_1, ..., G_{t-1}$),
- $t - 1$ scores $q(X|G_1, g), ..., q(X|G_{t-1}, g)$
- estimated edge-inclusion probabilities $Pr(\omega_{ij} \neq 0|G_1, ..., G_{t-1})$, $i, j = 1, ..., p$,

3 steps:

1. perform a stochastic local update to the graph based on edge-inclusion probabilities $\Rightarrow$ new graph $G_t$,
2. score the graph $\Rightarrow q(X|G_t, g)$,
3. update the edge-inclusion probabilities $\Rightarrow Pr(\omega_{ij} \neq 0|G_1, ..., G_t)$. 
Local update *via* 2 kinds of moves:

- **local moves**: choose randomly to add or delete an edge. If add, do so in proportion to their estimated edge-inclusion probabilities. If delete, do so in inverse proportion to them,

- **resampling step**: revisit one of \((G_1, ..., G_{t-1})\) in proportion to their score and make local move from the resampled graph.

Before SLS, good to initialize the search with a set of promising graphs for resampling.
### Initialization strategy using Neighborhood Fusion

- Neighborhood Fusion (NF) to quickly produce large sets of high quality GGM structures.

- In the space of conditional regressions,
  1. it exploits the sparse linear regression method LASSO through LARS algorithm [Tib96] to compute a set of candidate neighborhood structures for each variable,
  2. it specifies a mechanism for sampling and
  3. a mechanism for combining these neighborhoods to form undirected graphs.
Model choice

We consider

- the graph with the highest score among those explored,
- the *median probability model* $G_{\text{med}}$:

$$G_{\text{med}} = (V, E_{\text{med}}),$$

where $E_{\text{med}} = \{(i, j) : \Pr(\omega_{ij} \neq 0|G_1, \ldots, G_T) \geq 0.5\}$,

Choose it if its score is bigger and if it was not explored.
Portfolio: 27 energy products, called futures contracts, on the UK energy market.

Futures: contracts between two parties to exchange a specified commodity of standardized quantity and quality for a price agreed today with delivery occurring at a specified future date, the delivery date. Here 27 futures:

- 9 of different delivery periods on the Electricity market (1Month Ahead-2MAH-3MAH-1Quarter Ahead-2QAH-1Season Ahead-2SAH-3SAH-4SAH),

- 18 of different delivery periods on the Gaz market (1MAH-2MAH-3MAH-4MAH-5MAH-6MAH-7MAH-8MAH-9MAH-10MAH-11MAH-12MAH-13MAH-14MAH-15MAH-16MAH-17MAH-18MAH).

To understand futures...:
We apply our proposed model-selection procedure from 200 price returns in dimension 27. All the graphs are considered.

**Result**: matrix where element \( ij = 1 \) if \((i, j)\) is an edge of the selected graph.

| 1MAH | 2MAH | 3MAH | 1OAH | 2OAH | 1SAH | 2SAH | 3SAH | 1SAH | 2SAH | 1MAH | 2MAH | 3MAH | 1OAH | 2OAH | 1SAH | 2SAH | 3SAH | 1SAH | 2SAH | 1MAH | 2MAH | 3MAH | 1OAH | 2OAH | 1SAH | 2SAH | 3SAH | 1SAH | 2SAH | 1MAH | 2MAH | 3MAH |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| 0    | 1    | 1    | 0    | 1    | 0    | 0    | 0    | 1    | 1    | 0    | 1    | 0    | 1    | 0    | 1    | 1    | 0    | 1    | 1    | 0    | 0    | 0    | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    |
| 1    | 0    | 1    | 0    | 0    | 0    | 0    | 0    | 0    | 1    | 1    | 0    | 1    | 1    | 1    | 1    | 0    | 1    | 1    | 1    | 0    | 0    | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    |
| 1    | 1    | 0    | 1    | 0    | 1    | 0    | 0    | 1    | 0    | 0    | 0    | 0    | 0    | 1    | 0    | 0    | 0    | 1    | 0    | 0    | 0    | 0    | 0    | 0    | 0    | 1    | 1    | 1    | 1    | 1    | 1    | 1    |
| 1    | 0    | 1    | 0    | 1    | 1    | 1    | 0    | 0    | 0    | 0    | 0    | 0    | 0    | 0    | 0    | 1    | 1    | 0    | 0    | 0    | 0    | 1    | 0    | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    |
| 0    | 1    | 1    | 0    | 1    | 0    | 1    | 0    | 0    | 1    | 0    | 1    | 0    | 1    | 0    | 0    | 1    | 0    | 0    | 0    | 1    | 0    | 1    | 0    | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    |
| 1    | 0    | 0    | 1    | 1    | 0    | 1    | 1    | 0    | 1    | 0    | 0    | 1    | 0    | 1    | 0    | 1    | 0    | 0    | 0    | 1    | 0    | 1    | 0    | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    |
| 1    | 0    | 0    | 1    | 1    | 0    | 1    | 0    | 1    | 0    | 0    | 1    | 0    | 1    | 0    | 0    | 1    | 0    | 0    | 0    | 1    | 0    | 1    | 0    | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    |
| 0    | 1    | 1    | 0    | 1    | 0    | 0    | 1    | 0    | 0    | 1    | 1    | 0    | 1    | 1    | 1    | 0    | 1    | 1    | 1    | 0    | 0    | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    |
| 1    | 1    | 0    | 1    | 0    | 0    | 0    | 1    | 0    | 0    | 1    | 1    | 1    | 1    | 1    | 1    | 0    | 1    | 1    | 1    | 0    | 0    | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    |
| 0    | 1    | 1    | 0    | 1    | 0    | 0    | 1    | 0    | 0    | 1    | 1    | 1    | 1    | 1    | 1    | 0    | 1    | 1    | 1    | 0    | 0    | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    |

**Figure**: An idea of conditional-independence relationships between asset returns
• GGM: tractable model for covariance matrices in many dimensions and/or small samples + knowledge discovery.

• Study problem: estimation of the graph structure associated to a GGM.

• Main contributions: complete methodology to perform objective Bayesian model selection in general GGM - new objective matrix prior, properness condition for posterior, tools for model comparison and exploration of large model space.

• Perspective: estimation of the associated covariance matrix.
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