Learning Markov Equivalence Classes of Directed Acyclic Graphs: an Objective Bayesian Approach

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Outline

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- $\boldsymbol{y}_i = (y_{i,1}, \ldots, y_{i,q})^\top \quad i = 1, \ldots, n$
- $\boldsymbol{y}_i$s are i.i.d. from a parametric family of sampling distributions

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- Graph $\mathcal{G} = (V, E)$
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- Undirected graph (UG) graph with only directed edges
- Directed Acyclic Graph (DAG) graph with only directed edges (no cycles)
  - If the distributions of y_i exhibits conditional independencies determined by $\mathcal{D}$ (Markov wrt $\mathcal{D}$), then

$$f_{\mathcal{D}}(\boldsymbol{y}_i) = \prod_{j \in V} f\left(y_{i,j} \,|\, \boldsymbol{y}_{i,\mathrm{pa}_{\mathcal{D}}(j)}\right)$$

  - $\mathrm{pa}_{\mathcal{D}}(j)$ *parents* of node j in $\mathcal{D}$

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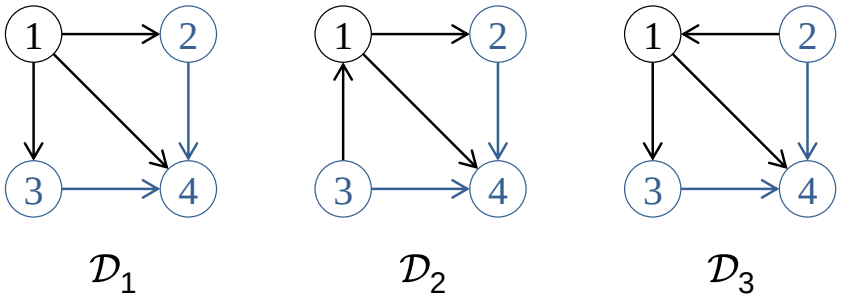
- Example: three Markov equivalent DAGs



Essential graph

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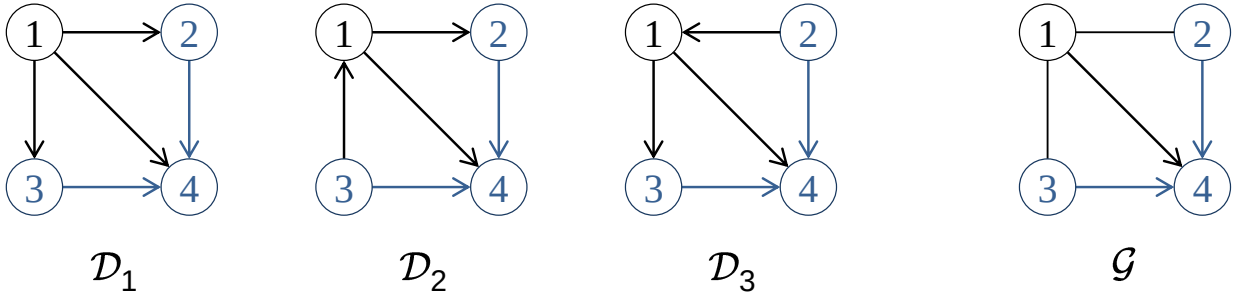

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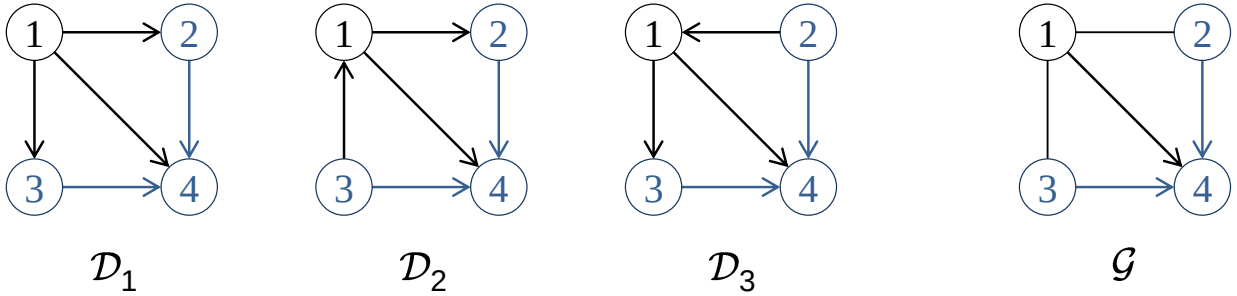

- $\mathcal{G}$ is a chain graph:
  - both directed and undirected edges
  - chain component: a set of nodes joined by an *undirected path*
  - $\mathcal{T}$: set of chain components of $\mathcal{G}$
  - $\mathcal{T} = \{\{1, 2, 3\}, \{4\}\}$

Essential graph (Characterization Theorem)

Theorem (Andersson et al., 1997)

A graph $\mathcal{G} = (V, E)$ is the EG for some DAG $\mathcal{D}$ with vertex set V if and only if $\mathcal{G}$ satisfies the following four conditions:

- *$\mathcal{G}$ is a CG;*
- *for each chain component $\tau \in \mathcal{T}$ the subgraph $\mathcal{G}_\tau$ is a decomposable UG;*
- *$\mathcal{G}$ has no flags (no induced subgraphs of the form $u \to v - z$);*
- *each directed edge $u \to v$ contained in $\mathcal{G}$ is strongly protected*

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  - cannot be naively used to compute marginal likelihoods

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$$m_{\mathcal{M}_k}(\boldsymbol{Y}; b) = \frac{\int f_{\mathcal{M}_k}(\boldsymbol{Y} \mid \boldsymbol{\theta}_k) p^D(\boldsymbol{\theta}_k) d\boldsymbol{\theta}_k}{\int f^b_{\mathcal{M}_k}(\boldsymbol{Y} \mid \boldsymbol{\theta}_k) p^D(\boldsymbol{\theta}_k) d\boldsymbol{\theta}_k}$$

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- Default choice: $b = n_0/n$, n_0 minimal (integer) training sample size which makes the induced fractional prior proper

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- Conditional density of variables in chain component τ

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- $\boldsymbol{\Gamma}_\tau$ matrix of regression parameters
- $\boldsymbol{\Omega}_{\mathcal{G}_\tau}$ (conditional) precision matrix
  Recall (Theorem 1) that $\boldsymbol{\Omega}_{\mathcal{G}_\tau}$ is Markov with respect to the decomposable graph $\mathcal{G}_\tau$.

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- Finally obtain the marginal likelihood of the essential graph $\mathcal{G}$ is

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- Then the probability of transition from $\mathcal{G} \in \mathcal{S}$ to $\mathcal{G}' \in \mathcal{S}$ is

$$p_{\mathcal{G},\mathcal{G}'} = \begin{cases} 1/|\mathcal{O}_{\mathcal{G}}| & \text{if } \mathcal{G}' \in \mathcal{S}, \\ 0 & \text{otherwise.} \end{cases}$$

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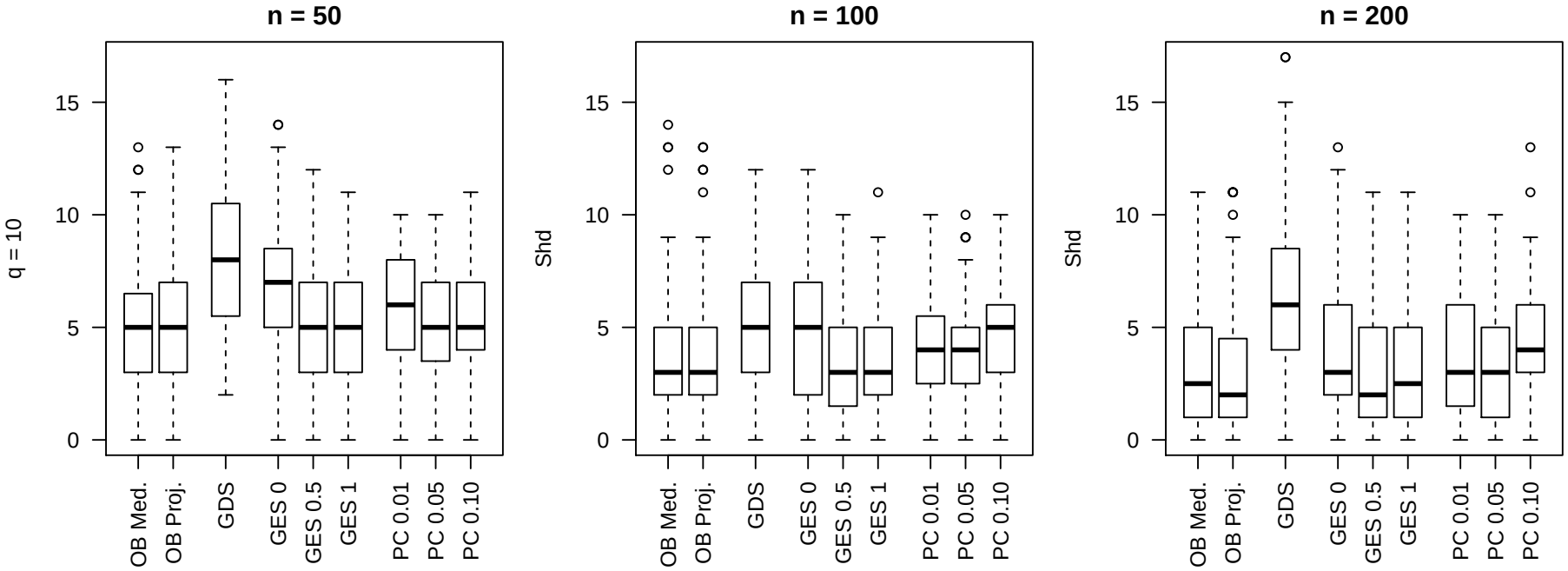
- We make a consistent extension of the PDAG and finally we obtain its EG named *projected median probability model*

Simulation setting

- Consider $q \in \{10, 20\}$, $n \in \{50, 100, 200\}$
- For each scenario (n, q) generate 50 datasets
- To obtain each dataset, randomly generate a DAG $\mathcal{D}$ on q nodes and simulate n i.i.d observations from $\mathcal{N}(\mathbf{0}, \mathbf{\Omega}_{\mathcal{D}}^{-1})$
- For each method (OBES and benchmarks) compute the Structural Hamming Distances between estimates and true EG over the 50 simulations

Results


n = 50
n = 100
n = 200
q = 10
Shd
Shd
0
5
10
15
OB Med.
OB Proj.
GDS
GES 0
GES 0.5
GES 1
PC 0.01
PC 0.05
PC 0.10

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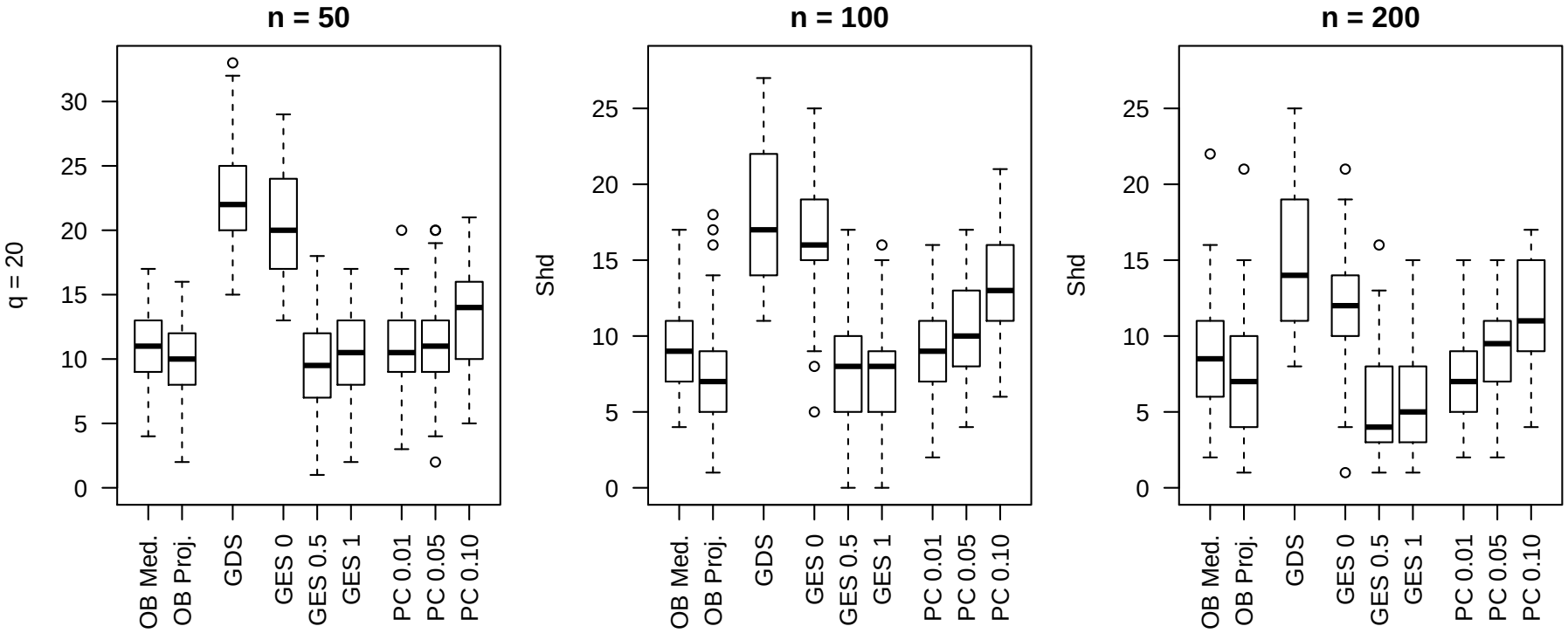
n = 50
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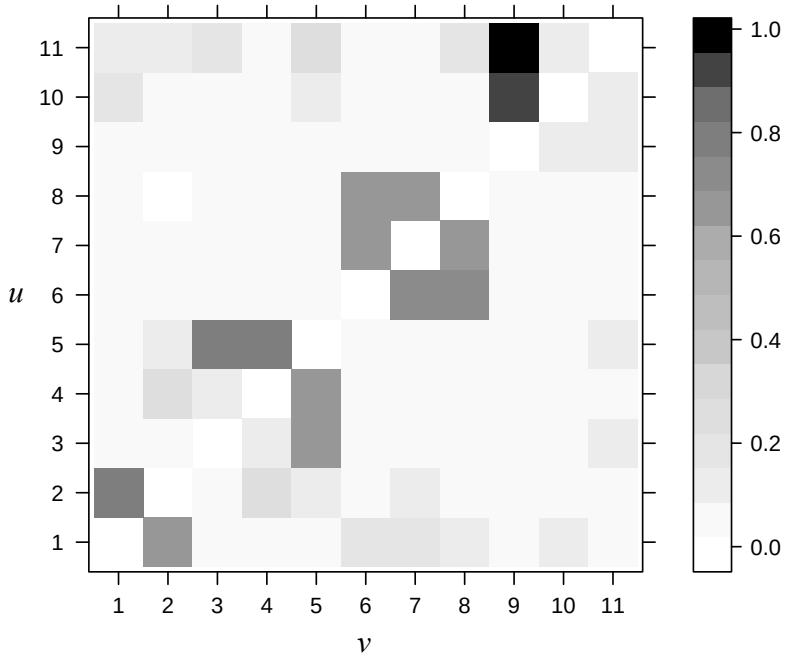
- We implement OBES on each dataset setting the maximum number of edges at 22) and running 10^5 MCMC iterations

Results (Dataset I)

- Heat map with posterior probabilities of edge inclusion $p_{u \to v}(\boldsymbol{Y})$



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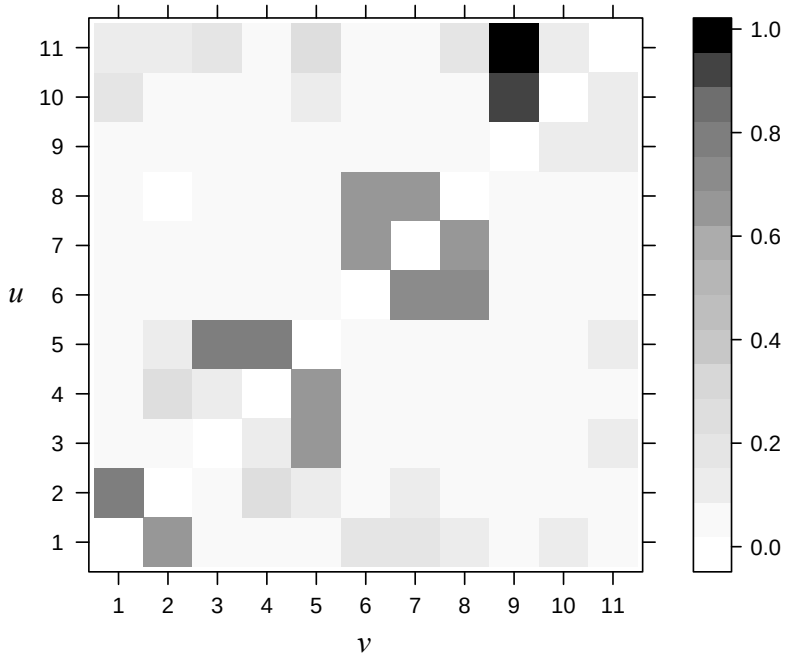

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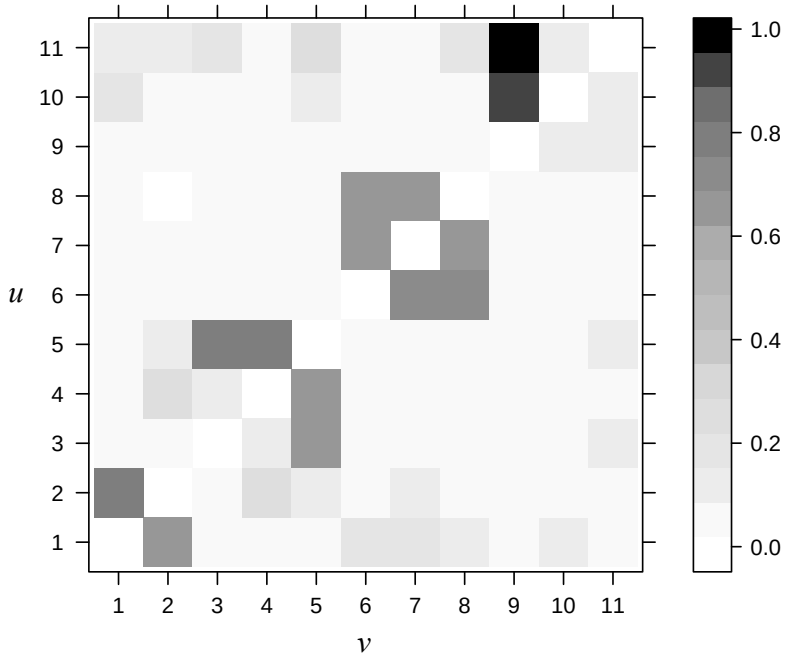

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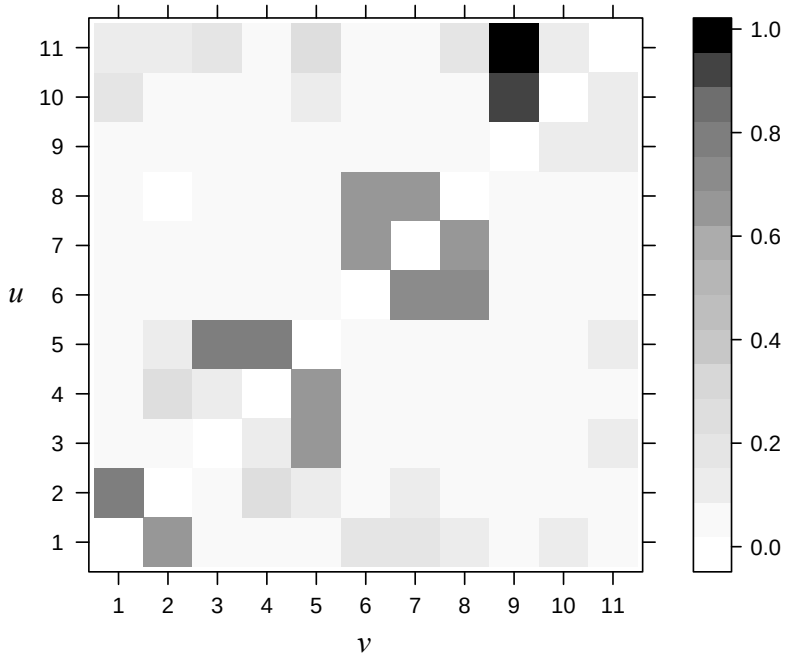

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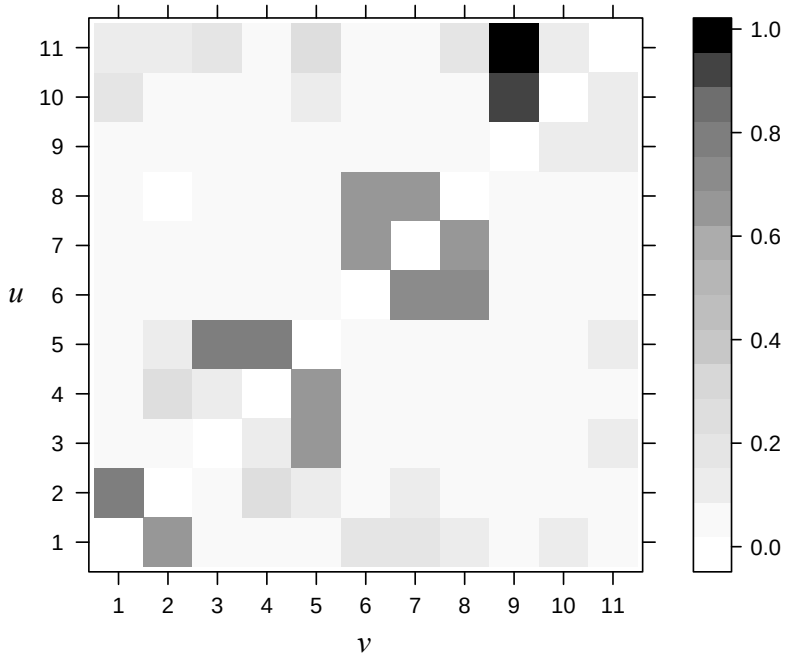

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- For comparison with benchmarks we construct the median probability graph model including all edges $u \to v$ such that $p_{u \to v} \geq 0.5$

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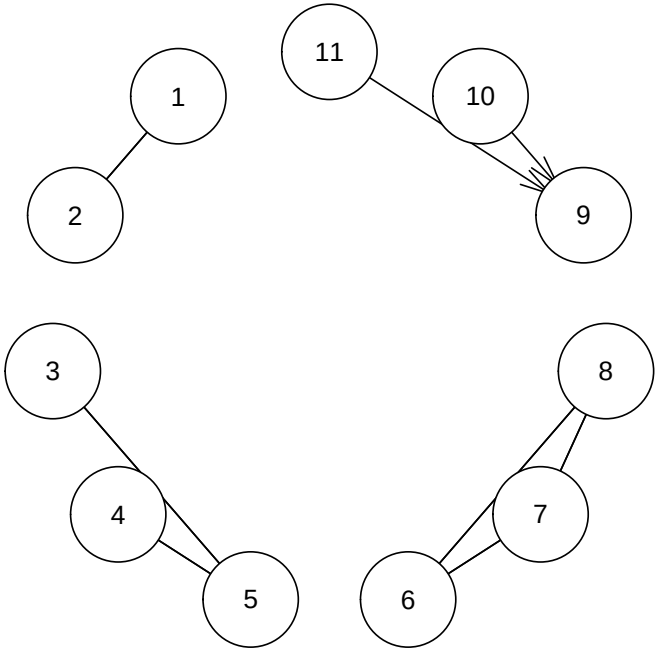
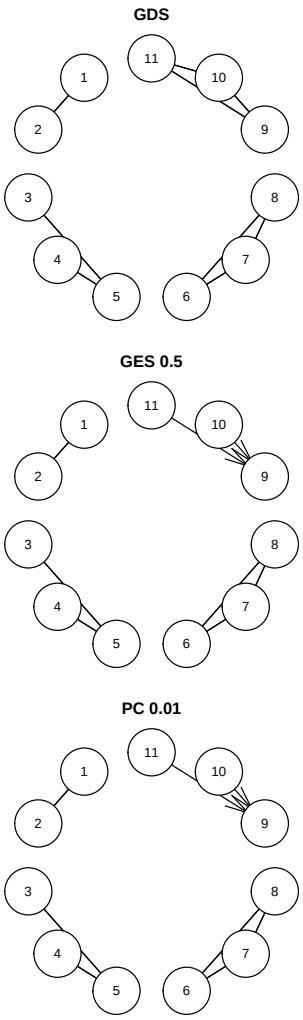
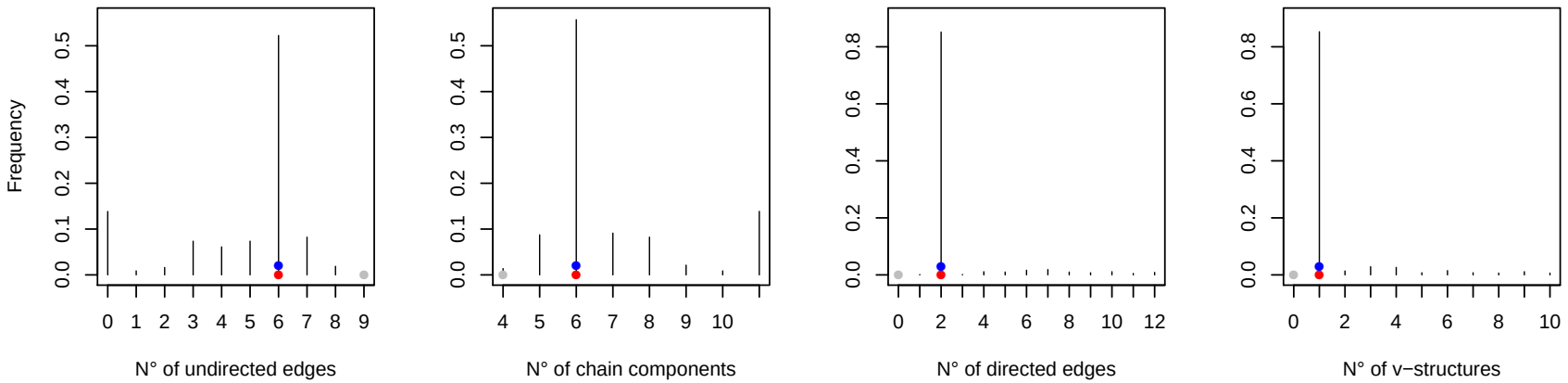


OBES median probability model



Results (Dataset I)

- Define the *quantile probability graph model* of order p^* as the graph including all edges $u \to v$ such that $p_{u \to v}(\boldsymbol{Y}) \geq p^*$



GDS (●), GES 0.5 (●), PC 0.01 (●)

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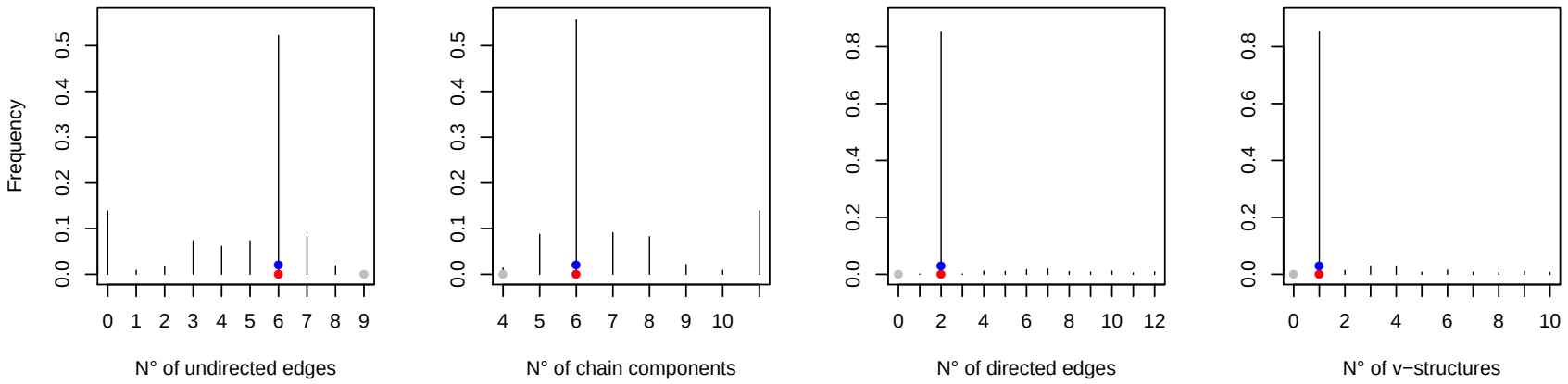

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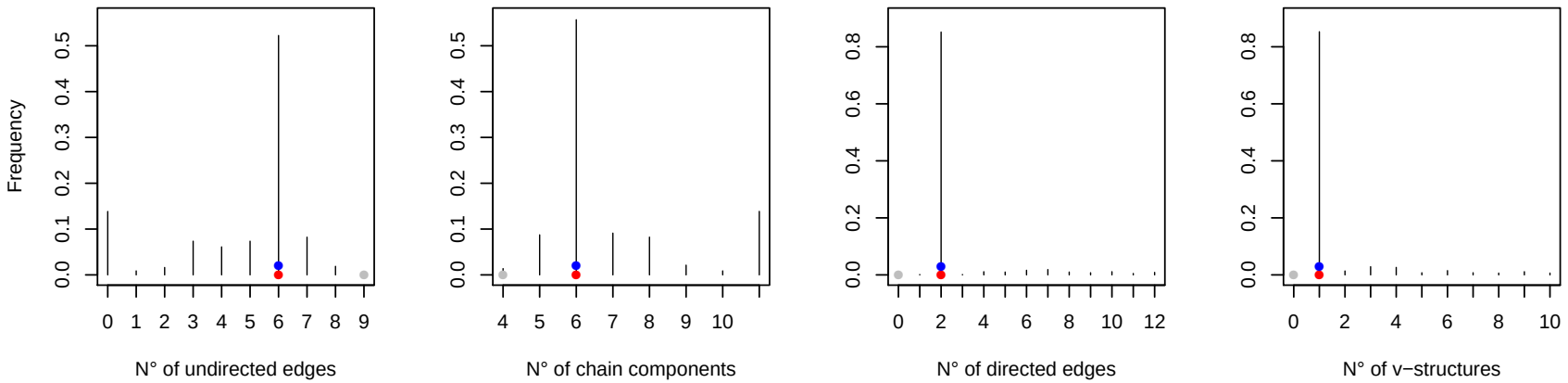
- For each graph choose a feature of interest (e.g number of directed edges) and obtain its frequency distribution by varying p^*



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- OBES is fully Bayes, and thus can provide an uncertainty evaluation of any feature of interest (e.g. the probability of inclusion of a particular edge) and not only a single estimate of the EG
- Being objective, it is virtually free from prior specifications

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  Extension to structural learning of *multiple* essential graphs with features potentially shared across graphs (Peterson et al., 2015)
- Extension of the methodology to jointly model *observational* and *interventional* data
  (produced under different exogenous perturbations of variables or by randomized intervention experiments) (Hauser & Bülmann, 2015)

Main references

ANDERSSON, S. A., MADIGAN, D. & PERLMAN, M. D. (1997).
A characterization of Markov equivalence classes for acyclic digraphs.
Ann. Statist. **25**, 505–541.

BHADRA, A. & MALLICK, B. K. (2013).
Joint high-dimensional Bayesian variable and covariance selection with an application to eQTL analysis.
Biometrics **69**, 447–457.

CARVALHO, C. & SCOTT, J. (2012).
Objective Bayesian model selection in Gaussian graphical models.
Biometrika **96**, 497–512.

CASTELO, R. & PERLMAN, M. D. (2004).
Learning essential graph Markov models from data.
In *Advances in Bayesian networks*, vol. 146 of *Stud. Fuzziness Soft Comput.* Springer, Berlin, 255–269.

CHICKERING, D. M. (2002).
Learning equivalence classes of Bayesian-network structures.
Journal of Machine Learning Research **2 (3)**, 445–498.

Main references

CONSONNI, G. & LA ROCCA, L. (2012).
Objective Bayes factors for Gaussian directed acyclic graphical models.
Scandinavian Journal of Statistics **39**, 743–756.

CONSONNI, G., La Rocca, L. & Peluso, S. (2017).
Objective Bayes Covariate-Adjusted Sparse Graphical Model Selection.
Scandinavian Journal of Statistics, **44**, 741–764.

DAWID, A. P. & LAURITZEN, S. L. (1993).
Hyper Markov laws in the statistical analysis of decomposable graphical models.
The Annals of Statistics **21**, 1272–1317.

GEIGER, D. & HECKERMAN, D. (2002).
Parameter priors for directed acyclic graphical models and the characterization of several probability distributions.
The Annals of Statistics **30**, pp. 1412–1440.

HAUSER, A. & BÜHLMANN, P. (2015).
Jointly interventional and observational data: estimation of interventional Markov equivalence classes of directed acyclic graphs.
Journal of the Royal Statistical Society B **77**, 291–318.

Main references

HE, Y., JIA, J. & YU, B. (2013).
Reversible MCMC on Markov equivalence classes of sparse directed acyclic graphs.
Ann. Statist. **41**, 1742–1779.

O'HAGAN, A. (1995).
Fractional Bayes factors for model comparison.
Journal of the Royal Statistical Society B **57**, 99–138.

PETERSON, C., STINGO, F. C. & Vannucci, M. (2015).
Bayesian inference of multiple Gaussian graphical models.
Journal of the American Statistical Association, **110 (509)**, 159–174.

SACHS, K., Perez, O., Pe'er, D., Lauffenburger, D. A. & Nolan, G. P. (2005).
Causal Protein-Signaling Networks Derived from Multiparameter Single-Cell Data.
Science, **308**, 523-529.

SPIRTES, P. AND GLYMOUR, C. AND SCHEINES, R. (2000).
Causation, Prediction and Search (2nd edition).
Cambridge, MA: The MIT Press., 1-16.

Supplementary slides

Gaussian multivariate regression DAGs

- Use theory developed in Consonni et al (2017) to perform objective Bayes learning for Gaussian multivariate regression DAG models
- They extend the methodology of Geiger and Heckerman (2002) for constructing compatible priors across DAG models
  - to the regression setting with covariate $\boldsymbol{X}$
  - to the objective Bayes setting
    (using the fractional Bayes factor)
  - Key ideas
    - Assign a prior on the *unconstrained* parameters for the *complete* DAG model
      (easy; can use standard conjugate matrix normal Wishart)
    - Show that the fractional prior belongs to the above conjugate family
    - Deduce the marginal distribution of Y_J with $J \subseteq V$ under the *complete* model
      (easy because of conjugacy)
    - If $\mathcal{G}$ is decomposable, marginal likelihood is

$$m_{\mathcal{G}}(\boldsymbol{Y} \mid \boldsymbol{X}) = \frac{\prod_{C \in \mathcal{C}} m(\boldsymbol{Y}_C \mid \boldsymbol{X})}{\prod_{S \in \mathcal{S}} m(\boldsymbol{Y}_S \mid \boldsymbol{X})}$$

    - Important: both $m(\boldsymbol{Y}_C)$ and $m(\boldsymbol{Y}_S)$ are in closed form and computed under the *complete* graph using standard priors
      (no need for hyper-Inverse Wishart of the like)

Properties of the Markov chain on EG space

- *validity*: the transition probability from $\mathcal{G}$ to $\mathcal{G}'$ that is not an EG is zero and the transition probability of an EG to itself is null

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  - update $\mathcal{G}_t = \mathcal{G}'$ with probability α, $\mathcal{G}_t = \mathcal{G}_{t-1}$ with probability $1 - \alpha$

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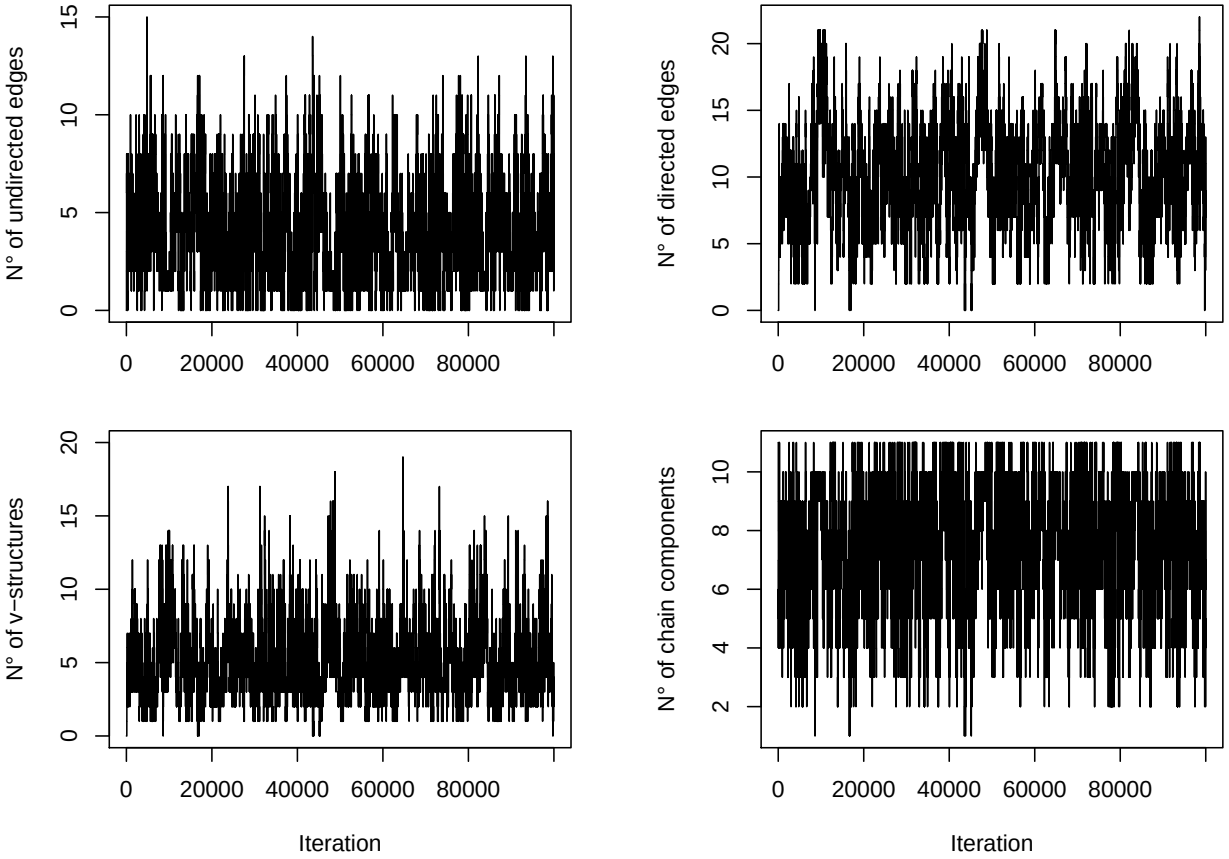
- Generate datasets of size n accordingly

Diagnostics (Dataset I)

- MCMC traceplots of some graph features for the visited graphs



Further slides

Possibly add condition on n and n_0

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  - $\boldsymbol{B}$ $(p+1) \times q$ matrix of unconstrained regression parameters
  - $\boldsymbol{\Omega}_{\mathcal{D}}$ $q \times q$ precision matrix, Markov with respect to a DAG $\mathcal{D}$

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- $p^F(\boldsymbol{B}, \boldsymbol{\Omega})$ is a matrix normal Wishart, which satisfies Geiger & Heckerman assumptions and produces a closed form expression for the marginal density of any (column) submatrix of $\boldsymbol{Y}$

Case 2) $\mathcal{D}$ not complete

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- $\mathcal{C}$ set of cliques
- $\mathcal{S}$ set of separators
- $\boldsymbol{Y}_C$ submatrix of responses belonging to $C \in \mathcal{C}$

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- $\boldsymbol{\Omega}_{\mathcal{G}}$ Markov with respect to a decomposable UG $\mathcal{G}$
- Marginal likelihood of $\mathcal{G}$

$$m_{\mathcal{G}}(\boldsymbol{Y} \,|\, \boldsymbol{X}) = \frac{\prod_{C \in \mathcal{C}} m(\boldsymbol{Y}_C \,|\, \boldsymbol{X})}{\prod_{S \in \mathcal{S}} m(\boldsymbol{Y}_S \,|\, \boldsymbol{X})}$$

- $\mathcal{C}$ set of cliques
- $\mathcal{S}$ set of separators
- $\boldsymbol{Y}_C$ submatrix of responses belonging to $C \in \mathcal{C}$
- $\boldsymbol{Y}_S$ submatrix of responses belonging to $S \in \mathcal{S}$

Case 2) $\mathcal{D}$ not complete

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- Important: $m(\boldsymbol{Y}_C)$ is computed under any *complete* graph using the matrix normal Wishart fractional prior (and similarly for $m(\boldsymbol{Y}_S)$)

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- Use (1) to obtain the marginal likelihood of an EG.

EG Chain component τ

Fractional prior

$$
\begin{aligned}
p^F(\boldsymbol{B}_\tau, \boldsymbol{\Omega}_\tau) \quad &\propto \quad |\boldsymbol{\Omega}_\tau|^{\frac{a_D + n_0 - |\mathrm{pa}_{\mathcal{G}}(\tau)| - |\tau| - 2}{2}} \\
&\cdot \quad e^{-\frac{n_0}{2}\mathrm{tr}\left(\boldsymbol{\Omega}_\tau \left\{ (\boldsymbol{B}_\tau - \hat{\boldsymbol{B}}_\tau)^\top \tilde{\boldsymbol{C}}_\tau \, (\boldsymbol{B}_\tau - \hat{\boldsymbol{B}}_\tau) + \tilde{\boldsymbol{R}}_\tau \right\}\right)},
\end{aligned}
$$

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\end{aligned}
$$

- $\hat{\boldsymbol{B}}_\tau = (\boldsymbol{X}_\tau^\top \boldsymbol{X}_\tau)^{-1} \boldsymbol{X}_\tau^\top \boldsymbol{Y}_\tau$

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$$

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- $\hat{\boldsymbol{E}}_\tau = (\boldsymbol{Y}_\tau - \boldsymbol{X}_\tau \hat{\boldsymbol{B}}_\tau)$

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EG Chain component τ

Fractional prior

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p^F(\boldsymbol{B}_\tau, \boldsymbol{\Omega}_\tau) \quad &\propto \quad |\boldsymbol{\Omega}_\tau|^{\frac{a_D + n_0 - |\mathrm{pa}_{\mathcal{G}}(\tau)| - |\tau| - 2}{2}} \\
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- $\tilde{\boldsymbol{C}}_\tau = n^{-1} \boldsymbol{X}_\tau^\top \boldsymbol{X}_\tau$
- $\tilde{\boldsymbol{R}}_\tau = n^{-1} \hat{\boldsymbol{E}}_\tau^\top \hat{\boldsymbol{E}}_\tau$

EG Chain component τ

Fractional prior

$$p^F(\boldsymbol{B}_\tau, \boldsymbol{\Omega}_\tau) \propto |\boldsymbol{\Omega}_\tau|^{\frac{a_D+n_0-|\mathrm{pa}_{\mathcal{G}}(\tau)|-|\tau|-2}{2}} \cdot e^{-\frac{n_0}{2}\mathrm{tr}\left(\boldsymbol{\Omega}_\tau\left\{(\boldsymbol{B}_\tau-\hat{\boldsymbol{B}}_\tau)^\top \tilde{\boldsymbol{C}}_\tau (\boldsymbol{B}_\tau-\hat{\boldsymbol{B}}_\tau)+\tilde{\boldsymbol{R}}_\tau\right\}\right)},$$

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- $\tilde{\boldsymbol{R}}_\tau = n^{-1}\hat{\boldsymbol{E}}_\tau^\top \hat{\boldsymbol{E}}_\tau$

- Matrix normal Wishart
  conjugate to the conditional sampling model in chain component τ

Marginal density of data submatrix in τ

$$
\begin{aligned}
m_\tau(\boldsymbol{Y}_{J,\tau} \mid \boldsymbol{X}_\tau) \quad &= \quad \pi^{-\frac{(n-n_0)|J|}{2}} \frac{\Gamma_{|J|}\left(\frac{a_D+n-|\mathrm{pa}_{\mathcal{G}}(\tau)|-1-|\bar{J}|}{2}\right)}{\Gamma_{|J|}\left(\frac{a_D+n_0-|\mathrm{pa}_{\mathcal{G}}(\tau)|-1-|\bar{J}|}{2}\right)} \\
&\cdot \quad \left(\frac{n_0}{n}\right)^{\frac{|J|(a_D+n_0-|\bar{J}|)}{2}} |\hat{\boldsymbol{E}}_{J,\tau}^\top \hat{\boldsymbol{E}}_{J,\tau}|^{-\frac{n-n_0}{2}}
\end{aligned}
$$

- $\bar{J} = \tau \setminus J$, $|\bar{J}| = |\tau| - |J|$

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