Objective Bayes Learning of Graphical Models

Guido Consonni
Università Cattolica del Sacro Cuore
Milan, Italy

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Joint work with
Luca La Rocca (Università di Modena e Reggio Emilia)
Stefano Peluso (Università Cattolica del Sacro Cuore - Milan)

Outline

Graphical models

Objective Bayes Model Selection

DAG-models

Compatible Parameter Priors

Marginal Likelihood

Covariate-adjusted graphical models

Experimental results

Graphs

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Graph $\mathcal{G}$

$\mathcal{G} = (V, E)$

V: set of vertices

E: set of edges

$|V| = q$

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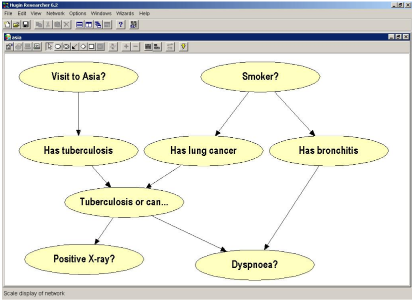

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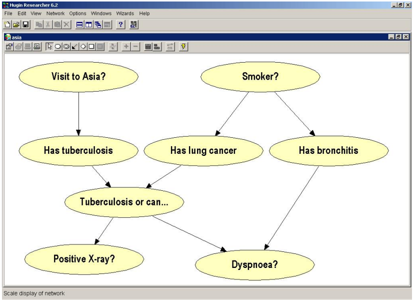

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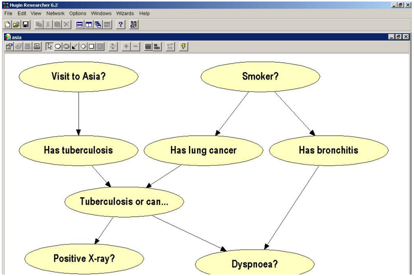

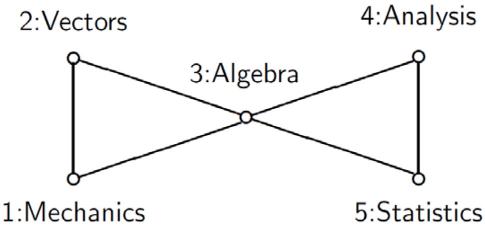

Graphical Models

When every edge in E is undirected, $\mathcal{G}$ is an undirected graph (UG).

When every edge in E is directed, $\mathcal{G}$ is a directed graph.

If a directed graph $\mathcal{G}$ has no directed cycles, then $\mathcal{G}$ is a DAG ($\mathcal{D}$).

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Given $\mathcal{G}$, a family of probability distributions for $\boldsymbol{y}_i^\top = (y_{i1}, \ldots, y_{iq})$ which factorize according to the graph $\mathcal{G}$ is called a graphical model (wrt $\mathcal{G}$).

Factorizations

If $\mathcal{G} = \mathcal{D}$ is a DAG

$$f_{\mathcal{D}}(\boldsymbol{y}_i \mid \boldsymbol{\theta}_{\mathcal{D}}) = \prod_{j=1}^{q} f(y_{ij} \mid \boldsymbol{y}_{i,\mathrm{pa}_{\mathcal{D}}(j)}, \boldsymbol{\theta}_j)$$

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$\mathcal{C}$: set of cliques; $\mathcal{S}$: set of separators.
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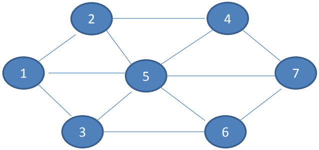

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$\mathcal{C} = \{\{1,2,5\},\{1,3,5\},\{2,4,5\},\{3,5,6\},\{4,5,7\},\{5,6,7\}\}$

$\mathcal{S} = \{\{1,5\},\{2,5\},\{3,5\},\{4,5\},\{5,6\}\}$

Markov properties

$\mathcal{G} \equiv \mathcal{D}$: DAG

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$\forall u \in V$

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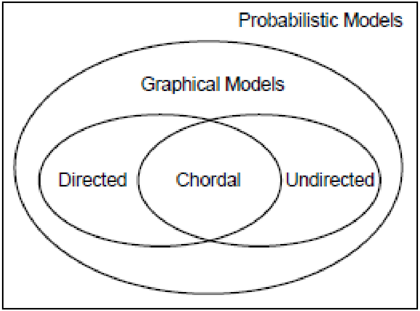
$\mathcal{G}$: UG
A, B, S disjoint subsets of V
Global Markov property
If S separates A from B in $\mathcal{G}$, then

$$A \perp\!\!\!\perp B \mid S$$

Relationships Among Graphical Models



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Graph selection

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$m_{\mathcal{M}_k}(\boldsymbol{Y}) = \int f_{\mathcal{M}_k}(\boldsymbol{Y} \mid \boldsymbol{\theta}_k) p(\boldsymbol{\theta}_k) d\boldsymbol{\theta}_k$
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Bayes factor for $\mathcal{M}_k$ against $\mathcal{M}_{k'}$

$$BF_{kk'}(\boldsymbol{Y}) = m_{\mathcal{M}_k}(\boldsymbol{Y}) / m_{\mathcal{M}_{k'}}(\boldsymbol{Y})$$

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Lack of substantive prior information
$p(\boldsymbol{\theta}_k) = p^D(\boldsymbol{\theta}_k)$
$p^D(\boldsymbol{\theta}_k)$: objective default (non-informative) prior
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Fractional Bayes Factor

$b = b(n)$, $0 < b < 1$: fraction of sample size n

Fractional marginal likelihood of model $\mathcal{M}_k$

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

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Fractional Bayes factor (FBF)

$$BF_{kk'}(\boldsymbol{Y}; b) = m_{\mathcal{M}_k}(\boldsymbol{Y}; b) / m_{\mathcal{M}_{k'}}(\boldsymbol{Y}; b)$$

Default choice: $b = n_0/n$
n_0: minimal (integer) training sample size

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  Example: Gaussian graphical model

$$\boldsymbol{y} \mid \boldsymbol{\mu}, \boldsymbol{\Omega}_{\mathcal{G}} \sim N(\boldsymbol{\mu}, (\boldsymbol{\Omega}_{\mathcal{G}})^{-1})$$

$\boldsymbol{\Omega}_{\mathcal{G}}$ Markov w.r.t. UG $\mathcal{G}$

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  $\boldsymbol{\Omega}_{\mathcal{G}}$ Markov w.r.t. UG $\mathcal{G}$
  $\boldsymbol{\Omega}_{\mathcal{G}}$ s.p.d.
  but also
  $(\boldsymbol{\Omega}_{\mathcal{G}})_{ij} = 0$ whenever there is no edge between i and j in $\mathcal{G}$
  constrained parameter space
  $p(\boldsymbol{\Omega}_{\mathcal{G}})$ must comply with this constraint

Building parameter priors under DAG-models

Collection of DAG-models
Joint sampling density under DAG-model $\mathcal{D}$

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- 3: *Likelihood modularity*
  If two DAGs $\mathcal{D}_1$ and $\mathcal{D}_2$ are such that $\mathrm{pa}_{\mathcal{D}_1}(j) = \mathrm{pa}_{\mathcal{D}_2}(j)$, they describe the same sampling family for node j

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Assumptions 1,2,3 satisfied in the multivariate Gaussian model $N_q(\boldsymbol{\mu}, \boldsymbol{\Omega}^{-1})$
Assumptions 4 and 5 satisfied with usual conjugate prior
$(\boldsymbol{\mu}, \boldsymbol{\Omega}) \sim \textit{Normal} - \textit{Wishart}$
under any complete DAG-model
and imposed under any other DAG-model to build the prior.

Outline

Marginal Lik DAG-models

If Assumptions 1-5 hold, then

$$
\begin{aligned}
m_{\mathcal{D}}(\boldsymbol{Y}) &\overset{(1)}{=} \prod_{j=1}^{q} \int p_{\mathcal{D}}(\boldsymbol{\theta}_j) \prod_{i=1}^{n} f_{\mathcal{D}}(y_{ij} \mid \boldsymbol{y}_{i,\mathrm{pa}_{\mathcal{D}}(j)}; \boldsymbol{\theta}_j) d\boldsymbol{\theta}_j \\
&\overset{(2)}{=} \prod_{j=1}^{q} \int p_{\mathcal{C}_j}(\boldsymbol{\theta}_j) \prod_{i=1}^{n} f_{\mathcal{C}_j}(y_{ij} \mid \boldsymbol{y}_{i,\mathrm{pa}_{\mathcal{C}_j}(j)}; \boldsymbol{\theta}_j) d\boldsymbol{\theta}_j \\
&\overset{(3)}{=} \prod_{j=1}^{q} \int p_{\mathcal{C}_j}(\boldsymbol{\theta}_j) f_{\mathcal{C}_j}(\boldsymbol{Y}_j \mid \boldsymbol{Y}_{\mathrm{pa}_{\mathcal{C}_j}(j)}; \boldsymbol{\theta}_j) d\boldsymbol{\theta}_j \\
&\overset{(4)}{=} \prod_{j=1}^{q} m_{\mathcal{C}_j}(\boldsymbol{Y}_j \mid \boldsymbol{Y}_{\mathrm{pa}_{\mathcal{C}_j}(j)}),
\end{aligned}
$$

$\mathcal{C}_j$ is any complete DAG such that $\mathrm{pa}_{\mathcal{C}_j}(j) = \mathrm{pa}_{\mathcal{D}}(j)$
(1) use global parameter independence
(2) use prior and likelihood modularity
(3) recall that $\boldsymbol{Y}_j = (\boldsymbol{y}_{ij};\ i = 1, \ldots, n)$
(4) by definition of $m_{\mathcal{C}_j}(\boldsymbol{Y}_j \mid \boldsymbol{Y}_{\mathrm{pa}_{\mathcal{C}_j}(j)})$

Marginal Lik DAG-models (ctd)

In conclusion

$$m_{\mathcal{D}}(\boldsymbol{Y}) = \prod_{j=1}^{q} m_{\mathcal{C}_j}(\boldsymbol{Y}_j \mid \boldsymbol{Y}_{\mathrm{pa}_{\mathcal{C}_j}(j)}) = \prod_{j=1}^{q} \frac{m_{\mathcal{C}_j}(\boldsymbol{Y}_{\mathrm{fa}_{\mathcal{C}_j}(j)})}{m_{\mathcal{C}_j}(\boldsymbol{Y}_{\mathrm{pa}_{\mathcal{C}_j}(j)})} = \prod_{j=1}^{q} \frac{m(\boldsymbol{Y}_{\mathrm{fa}_{\mathcal{D}}(j)})}{m(\boldsymbol{Y}_{\mathrm{pa}_{\mathcal{D}}(j)})},$$

$\mathrm{fa}_{\mathcal{D}}(j) = \mathrm{pa}_{\mathcal{D}}(j) \cup \{j\}$

$m(\cdot)$: marginal under any complete DAG-model

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Bottom line
Only one single parameter prior need be elicited
under any complete (i.e. unconstrained) model
Huge simplification

Marginal Lik DAG-models (ctd)

In conclusion

$$m_{\mathcal{D}}(\boldsymbol{Y}) = \prod_{j=1}^{q} m_{\mathcal{C}_j}(\boldsymbol{Y}_j \mid \boldsymbol{Y}_{\mathrm{pa}_{\mathcal{C}_j}(j)}) = \prod_{j=1}^{q} \frac{m_{\mathcal{C}_j}(\boldsymbol{Y}_{\mathrm{fa}_{\mathcal{C}_j}(j)})}{m_{\mathcal{C}_j}(\boldsymbol{Y}_{\mathrm{pa}_{\mathcal{C}_j}(j)})} = \prod_{j=1}^{q} \frac{m(\boldsymbol{Y}_{\mathrm{fa}_{\mathcal{D}}(j)})}{m(\boldsymbol{Y}_{\mathrm{pa}_{\mathcal{D}}(j)})},$$

$\mathrm{fa}_{\mathcal{D}}(j) = \mathrm{pa}_{\mathcal{D}}(j) \cup \{j\}$

$m(\cdot)$: marginal under any complete DAG-model

Bottom line
Only one single parameter prior need be elicited
under any complete (i.e. unconstrained) model
Huge simplification

Next all we need is being able to evaluate marginals of (column) subsets of the data matrix $\boldsymbol{Y}$

Score Equivalence

Markov equivalence class

Class of DAG-models embodying same conditional independencies

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  [A decomposable graph $\mathcal{G}$ always admits a DAG version $\mathcal{G}^{<}$]

Marginal Lik Decomposable Graphical Models

$\mathcal{C}$: set of cliques
$\mathcal{S}$: set of separators

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

$m(\cdot)$: marginal data distribution under any *complete* graph

Marginal Likelihood of a Gaussian DAG-model

$\boldsymbol{y}_i \,|\, \boldsymbol{\mu}, \boldsymbol{\Omega}, \mathcal{D} \overset{iid}{\sim} N_q(\boldsymbol{\mu}, \boldsymbol{\Omega}_{\mathcal{D}}^{-1})$; $i = 1, \ldots, n$
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If $(\boldsymbol{\mu}, \boldsymbol{\Omega}) \sim \textit{Normal} - \textit{Wishart}$
$p(\boldsymbol{\mu} \mid \boldsymbol{\Omega}) = N_q(\boldsymbol{\mu} \mid \boldsymbol{m}, (c\boldsymbol{\Omega})^{-1})$
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Closed-form expressions for $m(\boldsymbol{Y}_J)$ are available ($J \subset \{1, \ldots, q\}$)
Geiger & Heckerman (2002)
[corrections in Kuipers, Moffa & Heckerman (2014, *Ann. Statist.*)]
C. and La Rocca (2012, *Scand. J. Statist.*)

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for decomposable UGs
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Outline

Marginal Likelihood of a Multivariate Gaussian Regression DAG Model

Extension of the previous results to the regression setting
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Assume ($\boldsymbol{B}$) and Ω unrestricted. Prior

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Marginal likelihood of any regression DAG-model can be evaluated

Genetical Genomics Experiments

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Fractional Marginal Likelihood

Default prior on complete DAG

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Formula for $m_{\mathcal{G}}(\boldsymbol{Y})$ holds provided $n > p + |C|$, $C \in \mathcal{C}$
sparsity condition on regression and graphical structure

Recommended settings $a_D = q - 1$; $n_0 = p + 2$

Variable selection

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Under sparse regression
$p_\gamma << p_\star$

Joint variable and graph selection

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Hierarchical model

$$\begin{aligned}
\boldsymbol{Y} \,|\, \gamma, \mathcal{G} &\sim m_{\mathcal{G}}(\boldsymbol{Y} \,|\, \gamma) \\
\gamma_i \,|\, \omega_\gamma &\overset{iid}{\sim} Ber(\omega_\gamma); \quad i = 2, \ldots, p_\star + 1 \\
G_i \,|\, \omega_G &\overset{iid}{\sim} Ber(\omega_G); \quad i = 2, \ldots, q \cdot (q-1)/2 \\
\omega_\gamma &\sim U(0,1) \\
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Graphical models

Objective Bayes Model Selection

DAG-models

Compatible Parameter Priors

Marginal Likelihood

Covariate-adjusted graphical models

Experimental results

Two simulation settings

- *Sparse block*
  $n = 50$
  $q \in \{30, 60, 120\}$
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Parameter values generated as in the settings we compare our method to
In particular
Chen et al (2016)
Bhadra and Mallick (2013)

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- Graph structure
  G_i=0 for $i \leq q(q-1)/2-10$ and G_i=1 otherwise for $i > q(q-1)/2-10$
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- Elements of $\boldsymbol{X}$ from the second to last column are randomly drawn from $N(10, 1)$

Magnified block

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- Graph structure
  Fix a 50×50 adjacency matrix G^l as above
  Full G is block diagonal with G^l replicated three times

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  Full G is block diagonal with G^l replicated three times
  Corresponding $\mathbf{\Omega}_{\mathcal{G}}$ is block diagonal with the three blocks $\mathbf{\Omega}^l_{\mathcal{G}}$, $5\mathbf{\Omega}^l_{\mathcal{G}}$, $10\mathbf{\Omega}^1_{\mathcal{G}}$
  $\mathbf{\Omega}_{\mathcal{G}}$ has sequentially magnified signals
- Regression structure
  True γ produced by randomly choosing each predictor with probability 0.05 among $p_\star$ potential predictors

Comparison with state-of-the-art methods for covariate-adjusted graphical model selection

- Objective Fractional Bayes Factor
  OBFBF
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Measures of performance for graph selection (Adjacency matrix)

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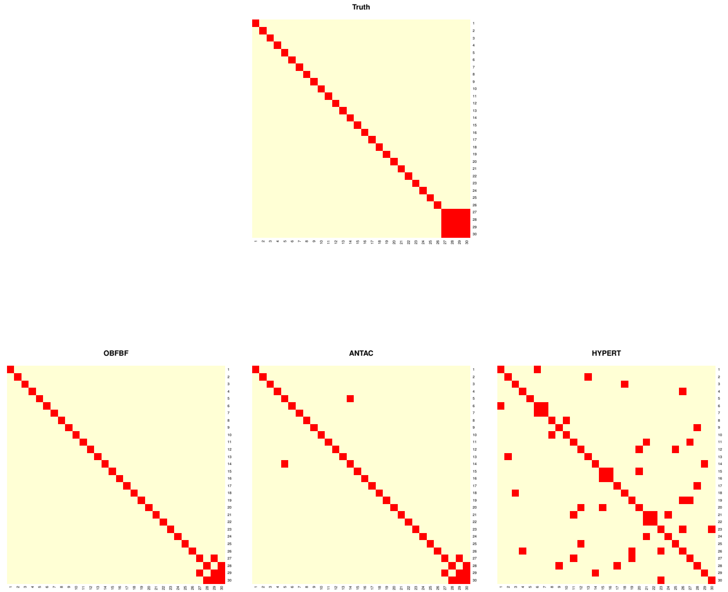
$$
\begin{aligned}
MISR &= \frac{FN + FP}{q(q-1)}, \quad SPE = \frac{TN}{TN + FP}, \\
SEN &= \frac{TP}{TP + FN} \\
MCC &= \frac{TP \cdot TN - FP \cdot FN}{\sqrt{(TP + FP)(TP + FN)(TN + FP)(TN + FN)}}
\end{aligned}
$$

Setting	(n, p^*, q)	Method	MISR	SPE	SEN	MCC	Time
Sparse	(50, 100, 30)	OBFBF	9(1)	92(1)	74(3)	47(5)	4769
		HYPERT	10(1)	91(1)	74(4)	46(2)	4270
		ANTAC	1(0)	100(0)	72(1)	84(1)	34
		GLASSO	83(5)	17(5)	86(4)	15(2)	8
		CONDIT	52(11)	48(11)	90(7)	21(4)	99
		LOWRANK	49(14)	50(14)	91(7)	22(5)	75
Sparse	(50, 100, 60)	OBFBF	3(2)	97(2)	84(1)	60(19)	5550
		HYPERT	5(0)	95(0)	84(2)	47(1)	5990
		ANTAC	0(0)	100(0)	83(1)	91(0)	109
		GLASSO	59(5)	41(5)	93(2)	12(1)	57
		CONDIT	27(19)	73(20)	89(4)	24(6)	268
		LOWRANK	81(3)	18(3)	97(3)	7(1)	236
Sparse	(50, 100, 120)	OBFBF	0(0)	100(0)	100(0)	95(5)	3745
		HYPERT	2(0)	98(0)	91(1)	54(1)	5941
		ANTAC	0(0)	100(0)	91(0)	95(0)	676
		GLASSO	36(4)	64(4)	95(1)	12(1)	547
		CONDIT	48(25)	52(25)	96(2)	11(5)	861
		LOWRANK	94(1)	6(1)	99(1)	1(0)	1002
Magnified	(50, 100, 150)	OBFBF	0(0)	100(0)	93(0)	92(12)	5498
		HYPERT	2(0)	99(0)	93(0)	54(1)	6770
		ANTAC	0(0)	100(0)	93(0)	96(0)	1971
		GLASSO	78(5)	22(5)	97(1)	5(1)	4570
		CONDIT	96(3)	4(3)	100(1)	2(1)	3517
		LOWRANK	98(0)	2(0)	100(0)	1(0)	5452

Sparse setting: $n = 200$, $p_\star = 100$, $q = 30$



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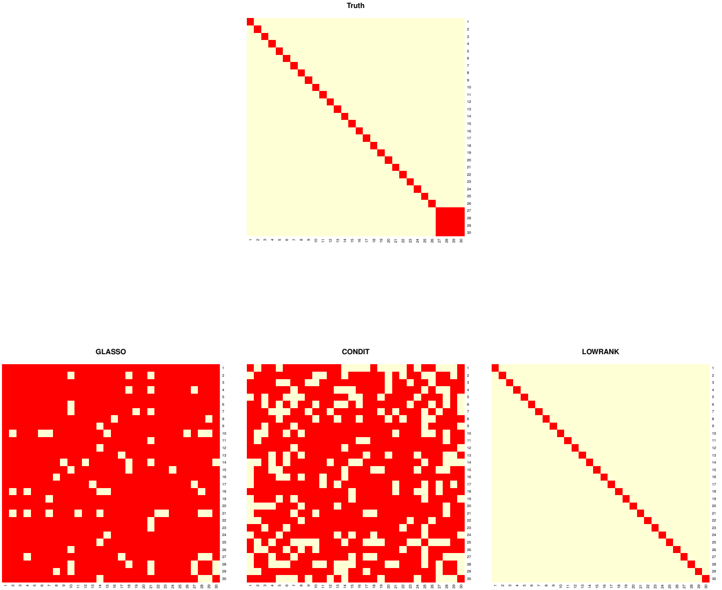

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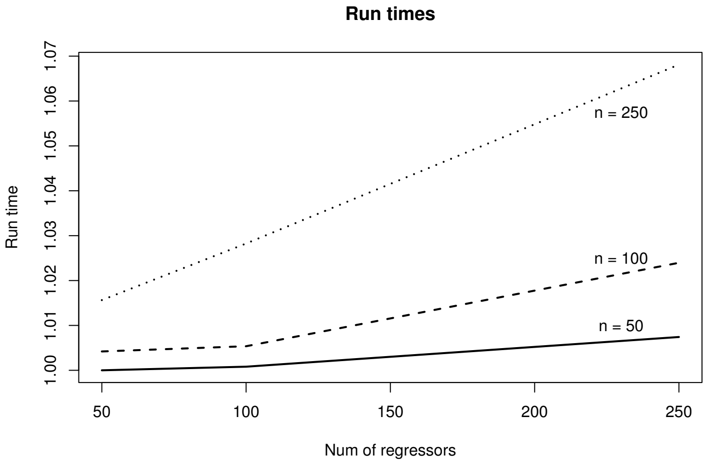
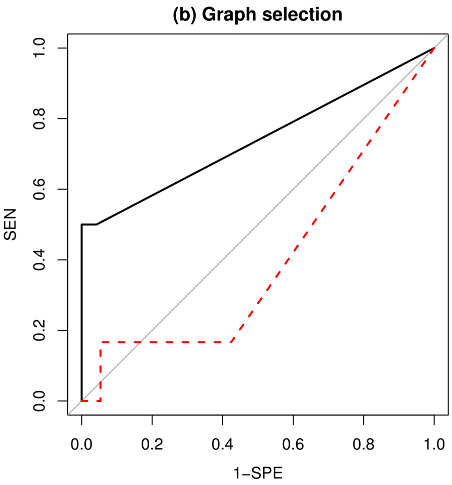
  However
  - *they perform also variable selection and return a richer output*
  - *Computational time for OBFBF increases only marginally (up to 7% from least to most complex setting)*

Runtimes for OBFBF

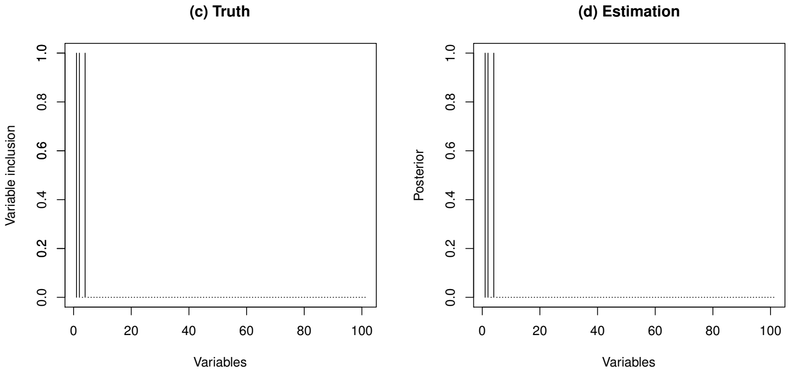


ROC curve: graph selection



Black: OBFBF
Red: HYPERT

Variable selection OBFBF



Conclusions I

Compatible parameter priors for the comparison of DAG-models can be constructed based on a single prior for the complete graph
(unconstrained parameter space)
Can use standard conjugate priors
Our contributions

- Objective Bayes (OB) method for comparing Gaussian DAG-models
  start with default prior
  and then apply the Fractional Bayes Factor

Conclusions II

- Covariate-adjusted OB method
  Joint graph and variable selection
  OBFBF comparable to ANTAC in graph selection for large and sparse networks
  although ANTAC does not perform variable selection explicitly
  OBFBF outperforms Bayesian competitor HYPERT as well remaining penalization-based methods
  OBFBF excellent performance in variable selection
  Computing time for MCMC-based methods higher but scales nicely with n, q and p

Looking ahead

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  Require calculations for Chain Graphs
  Use observational and interventional data

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