Graphical Gaussian Models with Symmetries and Regular Colourings

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Overview

1. Graphical Gaussian Models with Symmetries

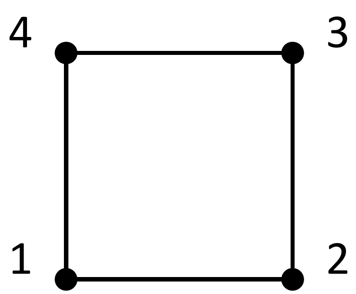
2. Need for Model Selection Methods Motivates Five Questions

3. Examples

Graphical Gaussian Models

- Concerned with the distribution of a multivariate Gaussian random vector
- Encode the independence structure in terms of edges in an undirected graph G=(V,E): vertices V = model variables, edges E defined by relation:

$$Y_\alpha \perp Y_\beta \mid Y_{V \setminus \{\alpha,\beta\}} \quad \Rightarrow \quad \alpha\beta \notin E$$



$$V = \{1,2,3,4\}$$
$$(Y_1, Y_2, Y_3, Y_4) \sim N_4(0, \Sigma)$$

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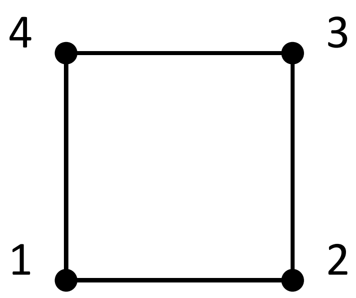

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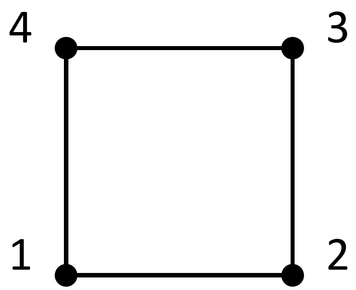

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$$\Sigma^{-1} = \begin{pmatrix} * & * & 0 & * \\ & * & * & 0 \\ & & * & * \\ & & & * \end{pmatrix}$$

positive definite

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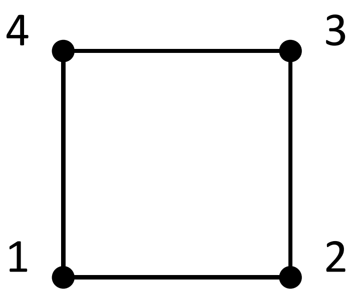
- If |V|=p, then there are up to |V|+|E| = p(p+1)/2 parameters in the model (for mean = 0)
- Parsimony in number of parameters can be achieved through
  - ... sparsity in graph
  - ... symmetry constraints on model parameters

Graphical Gaussian Models with Symmetries

- Højsgaard and Lauritzen (2008):
  - RCON models: equality constraints on concentrations
  - RCOR models: equality constraints on partial correlations



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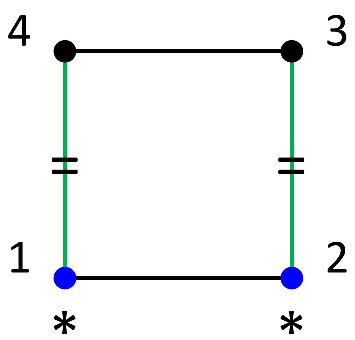

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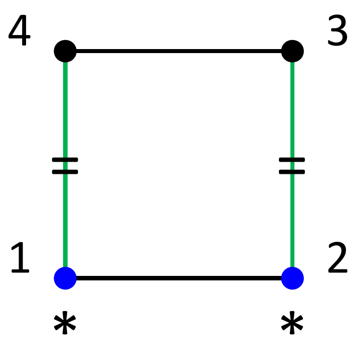

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$$c_{\alpha\beta} = -\rho_{\alpha\beta|V\setminus\{\alpha,\beta\}} = \frac{k_{\alpha\beta}}{\sqrt{k_{\alpha\alpha}k_{\beta\beta}}}$$

$$c_{14} = c_{23}$$

partial correlations

Graphical Gaussian Models with Symmetries

- Højsgaard and Lauritzen (2008):
  - RCON models: equality constraints on concentrations
    - Place linear constraints on natural parameter K of exponential family
    - Linear exponential families $\Longrightarrow$ MLE unique whenever it exists
  - RCOR models: equality constraints on partial correlations
    - Constrains not necessarily linear in natural parameter K
    - Curved exponential families $\Longrightarrow$ MLE not necessarily unique
    - Scale-invariance within vertex colour classes
  - MLE computation algorithms described in Højsgaard and Lauritzen (2008).

Graphical Gaussian Models with Symmetries

In order to make RCON and RCOR models widely applicable, model selection methods are required:

Q1: What is the structure of the set of RCON and RCOR models for a given V?

Q2: Can we design efficient model selection algorithms for RCON/RCOR models?

Q3: Are there statistically interesting model sub-classes?

Q4: If so, what is their structure?

Q5: Are they (better) suited for model selection?

RCON: symmetries in concentrations RCOR: symmetries in partial correlations

Q1: Structure of RCON and RCOR Models

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- Graphical representation: coloured graph = uncoloured graph + colouring
  - Obtain larger model through ...
    - ... larger uncoloured graph (fewer 0's in K)
    - ... finer colouring (fewer symmetries)
  - Can go from any model to any model:
    - Moving up: add edge colour classes + split colour classes
    - Moving down: drop edge colour classes + merge colour classes

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    - Can go from any model to any model:
        - Moving up: add edge colour classes + split colour classes
        - Moving down: drop edge colour classes + merge colour classes
    - Examining the graphical representation a bit closer: complete lattices!
        - Any two models have a unique supremum and infimum.
        - Smallest model = empty graph, all vertices same colour
        - Largest model = complete uncoloured graph

RCON: symmetries in concentrations

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Q2: Model Selection in RCON and RCOR Models

Q2: Can we design efficient model selection algorithms for RCON/RCOR models?

- Stepwise search theoretically possible however very large search space: $2^{|V|}$ uncoloured models on V, colouring enlarges model space considerably!

- Edwards-Havránek model selection procedure for lattices:
  - Whenever a model is accepted, all supermodels accepted.
  - Whenever a model is rejected, all submodels rejected.
  - Returns minimally accepted models.

- Possible .... but:
  - Model space still large.
  - Models not always intuitively interpretable: properties of found model(s)?

RCON: symmetries in concentrations

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Q3: Interesting Model Sub-Classes

Q3: Are there Statistically interesting model sub-classes?

RCON: symmetries in concentrations

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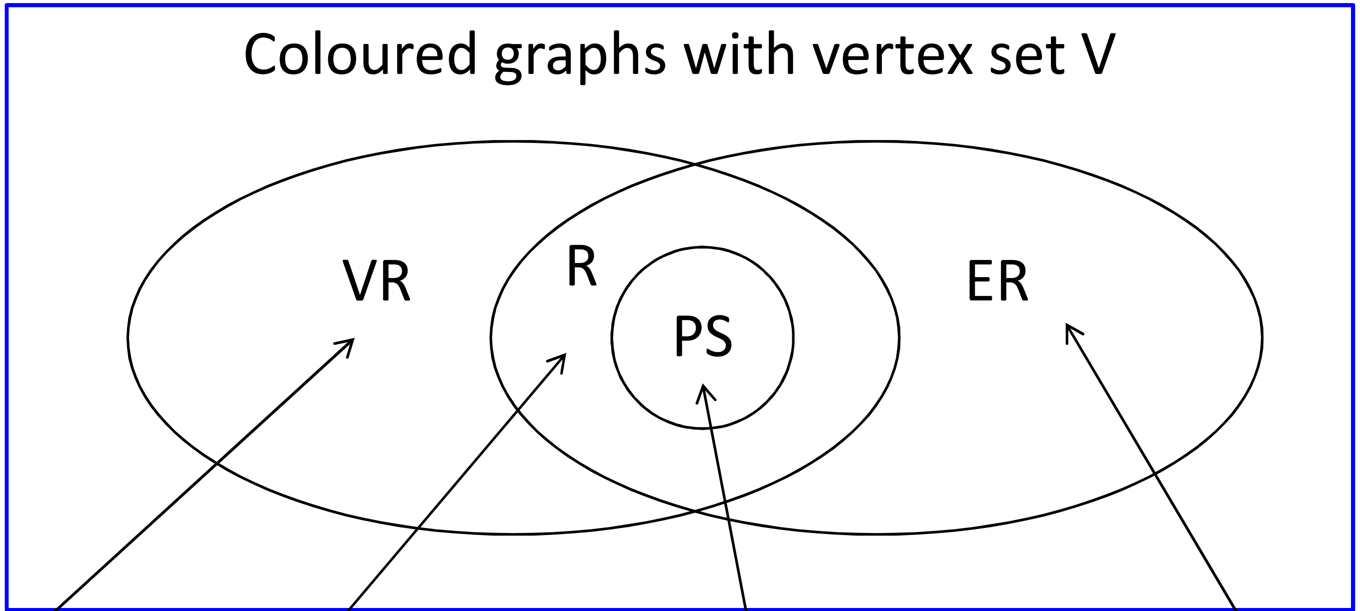
Q3: Interesting Model Sub-Classes

Q3: Are there Statistically interesting model sub-classes? YES!

They can be identified by their colouring:

(H&L, 2008; G&L, 2011)



Vertex regularity: estimability of mean

Regularity: vertex & edge regularity

Permutation symmetry: simplified MLE computation

Edge regularity: linear exponential families, scale-invariant (RCON = RCOR)

RCON: symmetries in concentrations

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Q4 & Q5: Structure of Model Sub-Classes

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RCON: symmetries in concentrations RCOR: symmetries in partial correlations

Q4 & Q5: Structure of Model Sub-Classes

Q4: If so, what is their structure?

- Each of ER, PG, VR and R is a complete lattice.
  - Any two models which lie in ER/PG/VR/R, they have unique infimum & supremum in the same model class. (non-trivial!)
  - Gehrmann (2011)

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Q5: Are they (better) suited for model selection? YES!

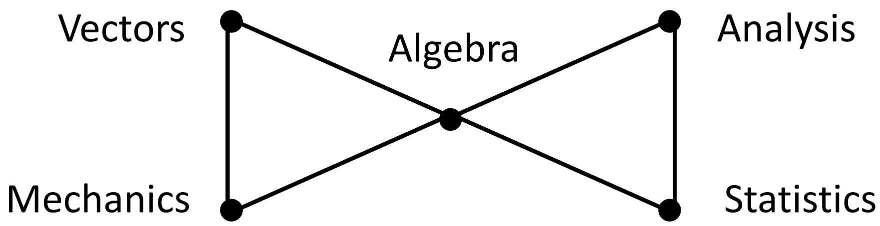
- Each model class qualifies for an Edwards-Havránek model search.
  - Faster than search in RCON/RCOR models.
  - Found model(s) guaranteed to have desirable properties.
  - Optionally: subsequent local search within RCON/RCOR models.

RCON: symmetries in concentrations RCOR: symmetries in partial correlations

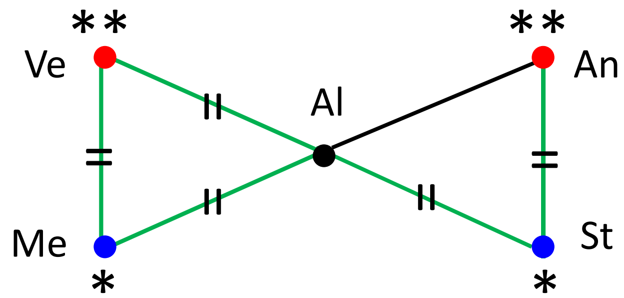
Example: Edge Regular Search

- Data: Examination marks of 88 students in 5 mathematical subjects (Mardia et al. 1979)

- Whittaker (1990) and Edwards (2000) :



- Højsgaard and Lauritzen (2008), RCON model:



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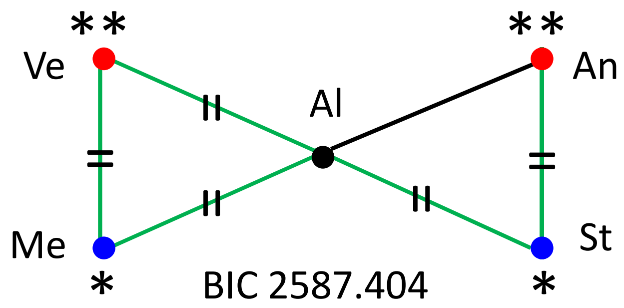
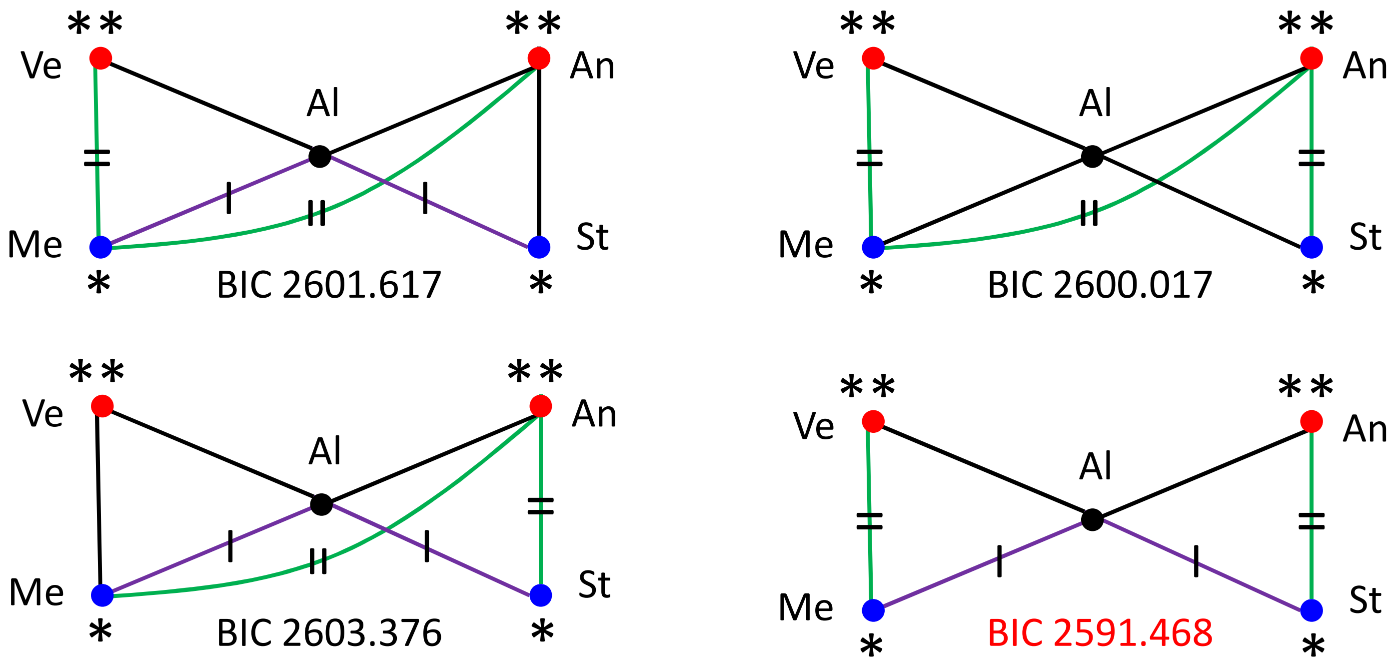


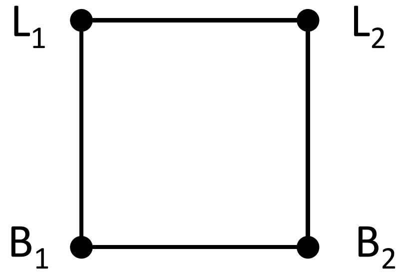
- Edwards-Havránek search, starting at saturated model, after 232 models:



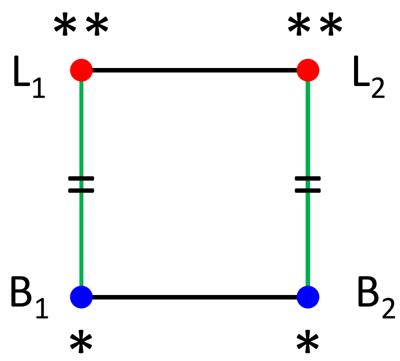
Example: Permutation Generated Search

- Data: Head dimensions of 25 pairs of 1st and 2nd sons, Frets (1921)

- Whittaker (1990):



- Højsgaard and Lauritzen (2008),
  RCOP model (permutation of sons):



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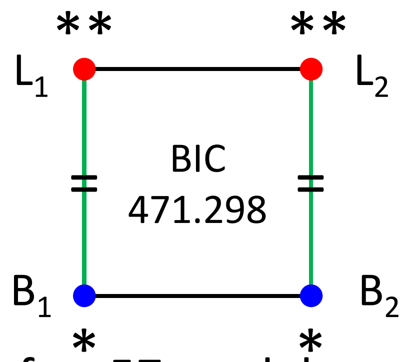
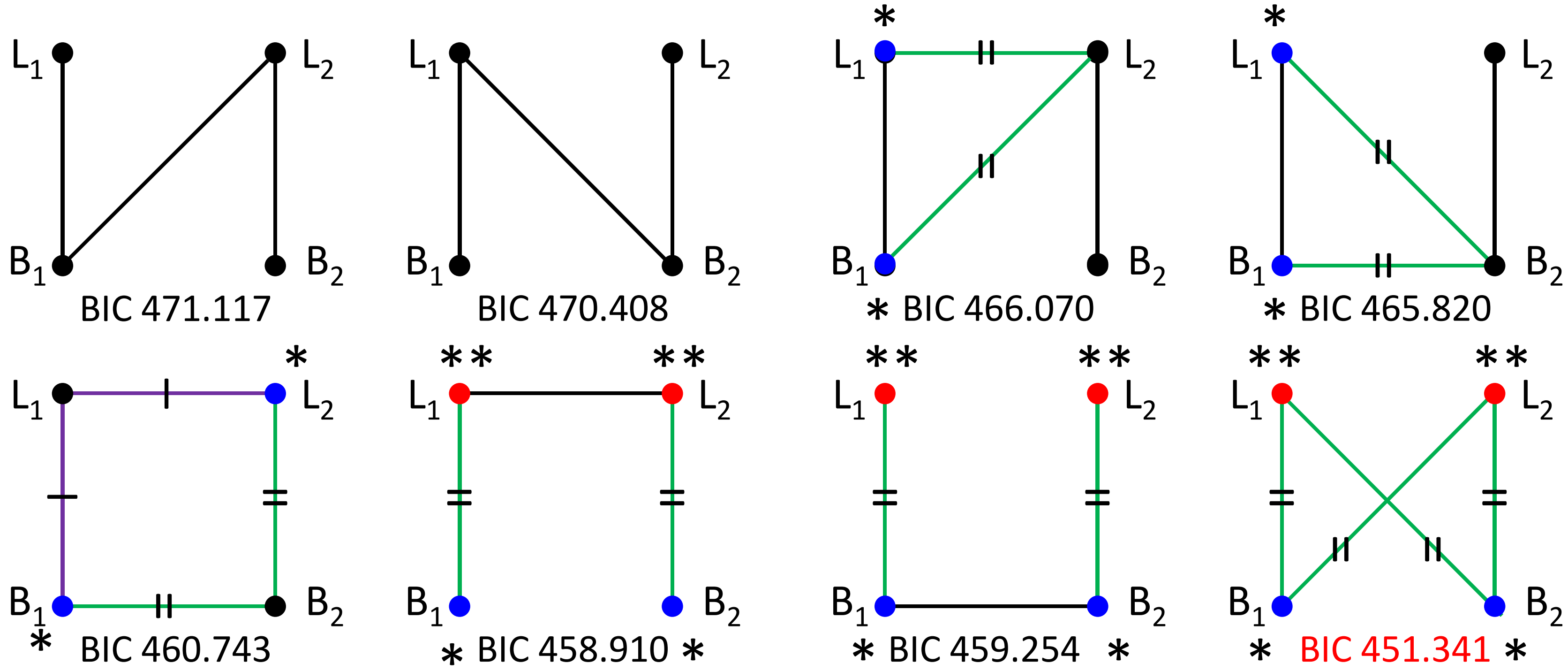


- Edward-Havránek search, starting at saturated model, after 57 models:



Summary

- Model selection in RCON and RCOR models can be performed by reducing search to lattices of models represented by regular colourings.
- These are first model selection procedures for GGMs with symmetries.
- Examples suggest that search may be feasible in general.
- Next step: full implementation and performance analysis.

Thank you!

References

Edwards, D. *Introduction to Graphical Modelling.* Springer Verlag: New York, NY, USA, 2000.

Edwards, D. and Havránek, T. A fast model selection procedure for large families of models. J*ournal of the American Statistical Association.* 1987, 82: 205-213.

Frets, G.P. Heredity of head form in man. *Genetica*. 1921, 41: 193-400.

Gehrmann, H. and Lauritzen, S.L. (2011). Estimation of means in graphical Gaussian models with symmetries. Preprint available at http://arxiv.org/abs/1101.3709.

Gehrmann, H. (2011) Lattices of graphical Gaussian models with symmetries. Preprint available at http://arxiv.org/abs/1104.1608.

Højsgaard, S. and Lauritzen, S.L. (2008). Graphical Gaussian models with edge and vertex symmetries. *Journal of the Royal Statistical Society Series B. 70: 1*005-1027.

Mardia, K. V., Kent, J. T. and Bibby, J. M. *Multivariate Analysis.* Academic Press: New York, NY, USA, 1979.

Whittaker, J. *Graphical Models in Applied Multivariate Statistics*. Wiley: Chichester, UK, 1990.