

# GAUSSIAN GRAPHICAL MODELS WITH MACAULAY2

ABSTRACT. Very brief introduction to mixed graphs and some of my early ideas

## 1. INTRODUCTION

We

## 2. GAUSSIAN MODELS OF MIXED GRAPHS

Following [5] we consider mixed graphs, that is graphs with undirected  $i - j$ , directed  $i \rightarrow j$  and bidirected edges  $i \leftrightarrow j$  but with no multiple edges between any two vertices. We assume that there is a partition of vertices  $U \cup W = V(G)$ , such that if  $i - j$  in  $G$  then  $i, j \in U$ , if  $i \leftrightarrow j$  in  $G$  then  $i, j \in W$  and there is no directed edge  $i \rightarrow j$  in  $G$  such that  $i \in W$  and  $j \in U$ . We assume that the subgraph on directed edges is acyclic. With all these assumptions on mixed graphs, we can order vertices in such a way that all vertices in  $U$  come before vertices in  $W$ , and whenever  $i \rightarrow j$  we have  $i < j$ . Note that we allow a pair of vertices to be connected by both a directed edge  $i \rightarrow j$  and bidirected edge  $i \leftrightarrow j$  or undirected edge  $i - j$ . With this setup, undirected graphs, DAGs, ancestral graphs [4] and chain graphs [1] occur as special cases.

Denote by  $\mathbb{R}^{V \times V}$  the set of matrices with rows and columns indexed by  $V$ , where vertices in  $V$  are ordered as described in the paragraph above. Let  $G = (V, E)$  be a mixed graph as defined above and let  $\mathbf{X} = (X_i)_{i \in V}$  be a Gaussian random vector with zero mean and covariance  $\Sigma \in \mathcal{S}_+^V$ , where  $\mathcal{S}_+^V$  is the set of symmetric positive definite matrices in  $\mathbb{R}^{V \times V}$ . We now introduce the family  $M(G) \subseteq \mathcal{S}_+^V$  of covariance matrices associated to  $G$ . We let  $\Lambda = [\lambda_{ij}] \in \mathbb{R}^{V \times V}$  to be a matrix such that  $\lambda_{ij} \neq 0$  only if  $i \rightarrow j$  in  $G$ . Next, we let  $K \in \mathcal{S}_+^V$  to be such that  $K_{ij} = 0$  if  $i - j \notin E$ . Similarly we let  $\Psi \in \mathcal{S}_+^V$  to be such that  $\Psi_{ij} = 0$  if  $i \leftrightarrow j \notin E$ . Given the three matrices  $\Lambda, K$  and  $\Psi$  described above we parametrize  $\Sigma \in M(G)$  by

$$(1) \quad \Sigma = (I - \Lambda)^{-T} \begin{bmatrix} K^{-1} & \mathbf{0} \\ \mathbf{0} & \Psi \end{bmatrix} (I - \Lambda)^{-1}.$$

In some situations it may be better to parametrize the covariance matrix  $K = \Sigma^{-1}$ . It is important to note that the parametrizations of covariance selection models and Gaussian Bayesian networks [3], Gaussian ancestral graph models [4] and chain graph models under the alternative Markov property [1] are all of the form given in (1).

Potentially interesting features:

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- **Geometry related:** generic identifiability, dimension, singular locus, check whether the ideal  $I_G$  of the model  $M(G)$  is determinantal
  - generic identifiability requires checking the rank of the Jacobian matrix at a generic point
  - the question if  $I_G$  is given by minors of  $\Sigma$  (or  $\Sigma^{-1}$ ) makes no sense for DAGs or undirected graphs because this is always true for these models
  - for mixed graphs this may be related to the trek ideal as described in [2]
- **Conditional independence related:** check if a mixed graph is Markov equivalent to an undirected (or purely bidirected) graph, check if two graphs are Markov equivalent
  - for the first, check if the ideal  $I_G$  is defined by vanishing some of the entries of the concentration matrix (or covariance matrix in the purely bidirected case) if yes, it would be nice to have as an output the corresponding undirected graph (with a note if it is chordal). This function should run routinely whenever we input a graph - it should stay in the silent mode in case there is no equivalence but should output a “warning” in case if such equivalence occurs.
  - for the second, check if two ideals are equal (after saturation)
- **Likelihood related:** ML-degree, check if a critical point is a local maximum, output the parameters mapping to  $\Sigma^*$ , sample covariance (not only data) as a possible input
- **Other** using predefined graph classes, imputing and visualizing graphs using package `visualize`, introduce different objects `MixedGraph`, `DirectedGraph`, `UndirectedGraph`. Also depending what is the graph structure the package could decide if it’s ‘better’ to work with covariance or concentration matrices.

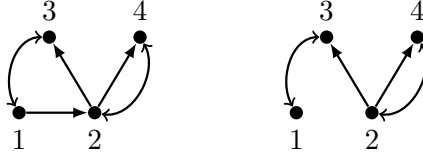
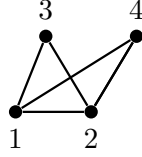


FIGURE 1. Two simple mixed graph models. The graph on the right is obtained from the one on the left by removing one arrow  $1 \rightarrow 2$ .

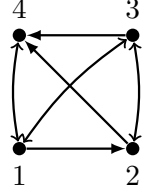
**Example 2.1.** Consider the graph given on the left of Figure 1.

- give basic characteristic
- singular locus
- introduce the `is.equivalent.undirected` feature
- maximum likelihood + closer analysis of the second critical point

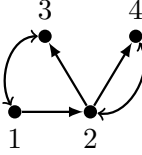
The model is Markov equivalent to the undirected graphical model given by the following graph



There are some other potential examples. The following graph should lead to a non-injective parametrization:



The following Seemingly Unrelated Regression model is equivalent to a DAG model...



#### REFERENCES

- [1] S. A. ANDERSSON, D. MADIGAN, AND M. D. PERLMAN, *Alternative Markov properties for chain graphs*, Scand. J. Statist., 28 (2001), pp. 33–85.
- [2] L. D. GARCÍA-PUENTE, S. PETROVIĆ, AND S. SULLIVANT, *Graphical models in macaulay2*, arXiv preprint arXiv:1208.6550, (2012).
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- [4] T. RICHARDSON AND P. SPIRITES, *Ancestral graph Markov models*, Ann. Statist., 30 (2002), pp. 962–1030.
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