Graphical Markov Models with Mixed Graphs in R

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Abstract

In this paper we provide a short tutorial illustrating the new functions in the package \mathbf{ggm} that deal with ancestral, summary and ribbonless graphs. These are mixed graphs (containing three types of edges) that are important because they capture the modified independence structure after marginalization over and conditioning on nodes of directed acyclic graphs. We provide functions to verify whether a mixed graph implies that A independent of B given C for any disjoint sets of nodes, and to generate maximal graphs inducing the same independence structure of non-maximal graphs. Finally, we provide functions to decide on the Markov equivalence of two graphs with the same node set but different type of edges.

1 Introduction and background

Graphical Markov models have become a part of the mainstream of statistical theory and application in recent years. These models use graphs to represent conditional independencies among sets of random variables. Nodes of the graph correspond to random variables and edges to some type of conditional dependencies.

Directed acyclic graphs. In the literature of graphical models the two most used classes of graphs are the directed acyclic graphs (DAGs) and the undirected graphs. DAGs have been proven useful, among other things, to specify the data generating processes when the variables satisfy an underlying partial ordering.

For instance, suppose that we have 4 observed variables Y, the ratio of systolic to diastolic blood pressure, X the diastolic blood pressure, both on log scale, Z, the body mass and W, the age, and that a possible generating process is the following linear recursive regression model

$$Y = \gamma_{YZ}Z + \gamma_{YU}U + \epsilon_{Y}$$

$$X = \gamma_{XW}W + \gamma_{XU}U + \epsilon_{X}$$

$$Z = \gamma_{ZV}W + \epsilon_{Z}$$

$$W = \epsilon_{W}; U = \epsilon_{U};$$

where all the variables are mean-centered and the ϵ s are zero mean, mutually independent Gaussian random errors. In this model we assume that there exist a genetic factor U influencing the ratio and levels of blood pressure.

Then, this model can be represented by the DAG in Figure 1(a) with nodes associated with the variables and edges, indicating the dependencies, represented by the regression coefficients γ s. From the graph it is seen for instance that the ratio of the two blood

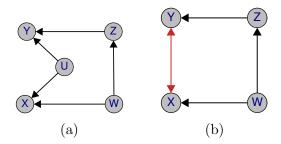


Figure 1: (a) A DAG; Y: (b) a regression graph.

pressures is directly influenced by body mass but not by age. Thus a consequence of the model is that the variables must satisfy a set of conditional independencies: for example the ratio of the blood pressure Y is independent of age W given body mass Z, written as $Y \perp \!\!\! \perp W \mid Z$.

A remarkable result is that the independencies can be deduced from the graph alone, without reference to the equations, by using a criterion called d-separation. In fact, in the graph of Figure 1(a), the nodes Y and W are d-separated given Z as can be checked using special graph algorithms included for example in packages **gRain** and **ggm**. For more details on DAG models and their implementation in R see the extensive discussion in Højsgaard et al. (2012).

Hidden variables and induced graphs The model has 4 observed variables but includes an unobserved variable, that is the genetic factor U. When U is hidden the model becomes

$$Y = \gamma_{YZ}Z + \eta_{Y}$$

$$X = \gamma_{XW}W + \eta_{X}$$

$$Z = \gamma_{ZV}W + \epsilon_{Z}$$

$$W = \epsilon_{W};$$

with two correlated errors $\eta_Y = \gamma_{YU}U + \epsilon_Y$ and $\eta_X = \gamma_{XU}U + \epsilon_X$, such that $\operatorname{cov}(\eta_Y, \eta_X) = \omega)YX$. As a consequence the model is still a recursive model and the parameters have a regression parameter interpretation, but contains some correlated residuals.

The induced model is said to be obtained after marginalization over U. In this model some of the original independencies are lost, but we can observe the implied independencies $Y \perp \!\!\! \perp W \mid Z$ and $X \perp \!\!\! \perp Z \mid W$. Also it can be shown that in a DAG model defined for the 4 observed variables is impossible to represent such independencies. Therefore, we say that DAG models are not stable under marginalization.

A mixed graph with arrows and arcs, shown in Figure 1(b) can however be used to represent the induced independence model after marginalization over U. In this representation, beside the arrows, represented by the γ s, we have the arc $Y \leftrightarrow X$ associated with the (partial) correlation ω_{YX} ,

The graph of Figure 1(b) belongs to a class of models called *regression chain graph* models. This class generalizes the recursive generating process of DAGs by permitting

joint responses, coupled in the graph by arcs, and thus appears an essential extension for applications.

The class of regression graphs is however itself not stable under marginalization. For instance, suppose that the generating process for the blood pressure data is defined by the more general regression chain graph of Figure 2(a) where L is a further variable representing a common hidden cause of systolic good pressure and body mass.

Then, after marginalization over L, the model can still be described by a a linear system of equations with correlated residuals and can be represented by the mixed graph shown in Figure 2(b). But the resulting graph is not a DAG nor a regression graph because it contains the pair of variables (Y, Z) coupled both by a directed edge and by a path composed by bi-directed arcs. Thus Y cannot be interpreted as a pure response to Z and in addition Y and Z are not two joint responses.

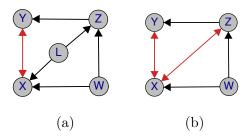


Figure 2: (a) A regression chain graph model; (b) the mixed graph obtained after marginalization over L is not a regression chain graph.

Stable mixed graphs. The previous illustrations show that when there are unobserved variables, DAG or regression chain graph models are no longer appropriate. The discussion could be extended to situations where there are some selection variables, that is hidden variables that are conditioned on.

This motivates the introduction of a more general class of *mixed graphs*, which contains three types of edge, denoted by lines, —, arrows, \rightarrow , and arcs (bi-directed arrows), \leftrightarrow . There are at least three known classes of mixed graphs without self loops that remain in the same class, i.e. that are *stable under marginalisation and conditioning*. The largest one is that of *ribbonless graphs* (RGs), (Sadeghi, 2012), defined as a modification of MC-graphs (Koster, 2002). Then, there is the subclass of *summary graphs* (SGs) (Wermuth, 2011), and finally the smallest class of the *ancestral graphs* (AGs) (Richardson and Spirtes, 2002).

Four tasks of the current paper. In this paper, we focus on the implementation of four important tasks performed on the class of mixed graphs in R:

- 1. Generating different types of stable mixed graphs after marginalisation and conditioning.
- 2. Verifying whether an independency of form $Y \perp \!\!\! \perp W | Z$ holds by using a separation criterion called *m*-separation.
- 3. Generating a graph that induces the same independence model as an input mixed graph such that the generated graph is *maximal*, i.e. each missing edge of the generated graph implies at least an independence statement.

4. Verifying whether two graphs are *Markov equivalent*, i.e. they induce the same independencies, and whether there is a Markov equivalent graph of a different type to an input graph of a specific type.

In the next section we give the details on how general mixed graphs are defined in package **ggm**. Next in each of the following sections we respectively deal with each of the tasks described above. For each task we give a brief introduction at the beginning of its corresponding section.

Package ggm. The previous tasks are illustrated by using a set of new functions introduced into the R package ggm. Some of the functions generalize previous contributions of ggm discussed in Marchetti (2006). Package ggm has been improved and it is now more integrated with other contributed packages related to graph theory, such as graph, igraph (Csardi and Nepusz, 2006), and gRbase (Dethlefsen and Højsgaard, 2005), which are now required for representing and plotting graphs. Specifically, in addition to adjacency matrices, all the functions in the package now accept graphNEL and igraph objects as input, as well as a new character string representation. A more detailed list of available packages for graphical models can be found at CRAN Task View gRaphical Models in R at http://cran.r-project.org/web/views/gR.html.

2 Defining mixed graphs in R

For a comprehensive discussion on the ways of defining a directed acyclic a graph, see (Højsgaard et al., 2012). A mixed graph is a more general graph type with at most three types of edge: directed, undirected and bi-directed, with possibly multiple edges of different types connecting two nodes. In **ggm** we provide some special tools for mixed graphs that are not present in other packages. Here we briefly illustrate some methods to define mixed graphs and we plot them with a new function, plotGraph, which uses a Tk GUI for basic interactive graph manipulation.

The first method is based on a generalization of the adjacency matrix. The second uses a descriptive vector and is easy to use for small graphs. The third uses a special function makeMG that allows to combine the directed, undirected and bi-directed components of a mixed graph.

Adjacency matrices for mixed graphs. In the adjacency matrix of a mixed graph we code the three different edges with a binary indicator: 1 for directed, 10 for undirected and 100 for bi-directed edges. When there are multiple edges the codes are added.

Thus the adjacency matrix of a mixed graph H with node set N and edge set F is an $|N| \times |N|$ matrix obtained as A = B + S + W by adding three matrices $B = (b_{ij})$, $S = (s_{ij})$ and $W = (w_{ij})$ defined by

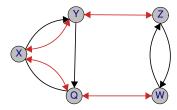
$$b_{ij} = \begin{cases} 1, & \text{if and only if } i \longrightarrow j \text{ in } H; \\ 0, & \text{otherwise.} \end{cases}$$

$$s_{ij} = s_{ji} = \begin{cases} 10, & \text{if and only if } i \longrightarrow j \text{ in } H; \\ 0, & \text{otherwise.} \end{cases}$$

$$w_{ij} = w_{ji} = \begin{cases} 100, & \text{if and only if } i \longleftrightarrow j \text{ in } H; \\ 0, & \text{otherwise.} \end{cases}$$

Notice that because of the symmetric nature of lines and arcs S and W are symmetric, whereas B is not necessarily symmetric.

For instance the following graph is a mixed graph (Notice that this mixed graph is not even ribbonless and hence of not much interest, and has been only introduced for presentation purposes):



that can be defined by the commands

```
> mg <- matrix(c( 0, 101,
                                       0, 110,
                                       0,
                   100,
                           0, 100,
                                             1,
                                             0,
                     0, 110,
                                 0,
                                       1,
                           0,
                                 1,
                                       0, 100,
                   110,
                           0,
                                 0, 100,
         5,5, byrow = TRUE)
> N <- c("X", "Y", "Z", "W", "Q")
> dimnames(mg) <- list(N, N)</pre>
> mg
    Х
              Ζ
         Y
                       Q
X
    0 101
              0
                   0 110
Y 100
         0 100
                       1
    0 110
              0
                       0
    0
                   0 100
W
         0
              1
              0 100
Q 110
         0
                       0
```

and plotted with plotGraph(mg).

Defining mixed graphs by using vectors. A more convenient way of defining small mixed graphs is based on a simple vector coding as follows. The graph is defined by a character vector of length 3f, where f = |F| is the number of edges, and the vector contains a sequence of triples $\langle \text{type}, \text{label1}, \text{label2} \rangle$, where the type is the edge type and label1 and label2 are the labels of the two nodes. The edge type accepts "a" for an directed arrow, "b" for an arcs and "l" for a line. Notice that isolated nodes may not be created by this method. For example, the vector representation of the previous mixed graph is

Once again as in the DAG case we can use plotGraph(mgv) to plot the defined graph.

Mixed graph using the function makeMG. Finally the adjacency matrix of a mixed graph may be built up with the function makeMG. This function requires three arguments dg, ug and bg, corresponding respectively to the three adjacency matrices B, S and W composing the mixed graph. These may also be obtained by the constructor functions DG and UG of ggm for directed and undirected graphs respectively. Thus for the previous mixed graph we can issue the command

```
> mg \leftarrow makeMG(dg = DG(Y^X, Z^W, W^Z),

ug = UG(^X*Q),

bg = UG(^Y*X + X*Q + Q*W + Y*Z))
```

obtaining the same adjacency matrix (up to a permutation).

3 Generating stable mixed graphs

There are four general classes of stable mixed graphs.

Ribbonless graphs are mixed graphs without a specific set of subgraphs called ribbons. The lack of ribbons ensures that, for any RG, there is a DAG whose independence structure, i.e. the set of all conditional independence statements that it induces, after marginalisation over and conditioning on two disjoint subsets of its node set can be represented by the given RG. This is particularly essential as it shows that the independence structures corresponding to RGs are probabilistic, that is there exists a probability distribution P that is faithful with respect to any RG, i.e. for random vectors X_A , X_B , and X_C with probability distribution P, $X_A \perp \!\!\!\perp X_B \mid X_C$ if and only if $\langle A, B \mid C \rangle$ is in the induced independence structure by the graph. This probability distribution is the marginal and conditional of a probability distribution that is faithful to the generating DAG.

Summary graphs have neither arrowheads pointing to lines (i.e. $\leftrightarrow \circ$ — or $\rightarrow \circ$ —) nor directed cycles with all its arrows pointing towards one direction. Ancestral graphs have these two constraint together with an additional constraint that these graphs do not contain so-called *bows*, see Richardson and Spirtes (2002).

However, notice that for some ribbonless and summary graphs the corresponding parametrisation is sometimes not available even in the case of standard joint Gaussian distribution.

If we suppose that stable mixed graphs are only used to represent the independence structure after marginalisation and conditioning, we can consider all types as equally appropriate. However, each of the three types has been used in different context and for different purposes. RGs have been introduced in order to straightforwardly deal with the problem of finding a class of graphs that is closed under marginalisation and conditioning by a simple process of deriving them from DAGs. SGs are used when the generating DAG is known and to trace the effects in the sets of regressions as described above. AGs are simple graphs, meaning that they do not contain multiple edges and the lack of bows ensures that they satisfy many desirable statistical properties.

In addition, when one traces the effects in regression models with latent and selection variables (as described in the introduction) ribbonless graphs are more alerting to possible distortions (due to indirect effects) than summary graphs, and summary graphs are more alerting than ancestral graphs; see also Wermuth and Cox (2008). For the exact definition and a thorough discussion of all such graphs, see Sadeghi (2012).

Sadeghi (2012) also defines the algorithms generating stable mixed graphs of a specific type for a given DAG or for a stable mixed graphs of the same type after marginalisation

and conditioning such that they induce the marginal and conditional DAG-independence structure. We implement these algorithms in this paper.

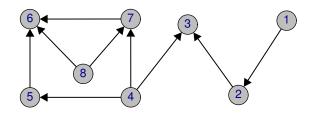
By "generating graphs" we mean applying the defined algorithms, e.g. those for generating stable mixed to graphs, in order to generate new graphs.

Functions to generate the three main types of stable mixed graphs. Three main functions RG, SG, and AG are available to generate and plot ribbonless, summary, and ancestral graphs from DAGs, using the algorithms in Sadeghi (2012). These algorithms look for the paths with three nodes and two edges in the graph whose inner nodes are being marginalized over or condition on, and generate appropriate edges between the endpoints. These have two important properties: (a) they are well-defined in the sense that the process can be performed in any order and produces always the same final graph; (b) the generated graphs induce the modified independence structure after marginalization and conditioning; see Sadeghi (2012) for more details.

The functions RG, SG, and AG all have three arguments: a the given input graph, M, the marginalization set and C, the conditioning set. The graph may be of class "graphNEL" or of class "igraph" or may be represented by a character vector, or by an adjacency matrix, as explained in the previous sections. The sets M and C (default c()) must be disjoint vectors of node labels, and they may possibly be empty sets. The output is always the adjacency matrix of the generated graph. There are two additional logical arguments showmat and plot to specify whether the adjacency matrix must be explicitly printed (default TRUE) and the graph must be plotted (default FALSE).

Some examples. We start from a DAG defined in two ways, as an adjacency matrix and as a character vector:

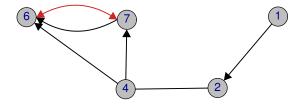
> plotGraph(ex)



Then we define two disjoint sets M and C to marginalize over and condition on

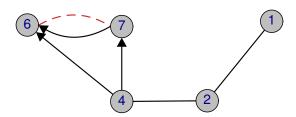
and we generate the ribbonless, summary and ancestral graphs from the DAG with the associated plot.

> RG(ex, M, C, plot = TRUE)



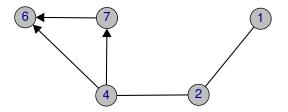
The summary graph is plotted with dashed undirected edges instead of bi-directed edges:

> plotGraph(SG(ex,M,C), dashed = TRUE)



The induced ancestral graph is obtained from the DAG defined as a vector.

> AG(exvec,M,C,showmat=FALSE, plot=TRUE)



4 Verifying m-separation

In general, a path is said to be m-connecting given C if all its collider nodes are in C or in the set of ancestors of C, and all its non-collider nodes are outside C. For two disjoint subsets of the node set A and B, we say that C m-separates A and B if there is no m-connecting path between A and B given C. This separation criterion has been implemented in R and the related function is provided in $\operatorname{\mathbf{ggm}}$.

Examples. The fundamental way to verify if a graphical model implies an independence $A \perp \!\!\!\perp B \mid C$ is to test whether the disjoint subsets A and B of the node set are m-separated given a third set C, and this may be done with the function msep. Note that there is still a function dSep in ggm for d-separation, although it is superseded by msep.

The function has 4 arguments, where the first is the graph a, in one of the forms discussed before, and the other three are the disjoint sets A, B and C. For example, consider the DAG of Figure 1(a):

```
> a < DAG(Y \sim U + Z, X \sim U + W, Z \sim W)
```

Then, we see that Y and W are m-separated given Z:

```
> msep(a,"Y","W","Z")
```

[1] TRUE

and the same statement holds for the induced ancestral graph after marginalization over U:

```
> b <- AG(a, M = "U")
> msep(b,"Y","W","Z")
```

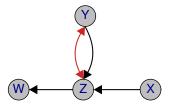
[1] TRUE

This was expected because the induced ancestral graph respects all the m-separation statements present in the DAG, and not involving the variable U.

As a more complex example, consider the following mixed graph,

```
> a <- makeMG(dg= DG(W \sim Z, Z \sim Y + X),
bg= UG(\sim Y*Z))
```

> plotGraph(a)



Then, the two following statements verify whether X is m-separated from Y given X, and whether X is m-separated from Y (given the empty set):

```
> msep(a,"X","Y","Z")
[1] FALSE
> msep(a,"X","Y")
[1] TRUE
```

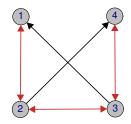
In this example m-separation is equivalent to its special case, the d-separation criterion for DAGs.

5 Verifying maximality

While for many subclasses of graphs a missing edge corresponds to some independence statement, for the more complex classes of mixed graphs this is not necessarily true. A graph where each of its missing edges is related to an independence statement is called a maximal graph. For a more detailed discussion on maximality of graphs and graph-theoretical conditions for maximal graphs, see Richardson and Spirtes (2002) and Sadeghi and Lauritzen (2011). Sadeghi and Lauritzen (2011) also gave an algorithm for generating maximal ribbonless graphs that induce the same independence structure to an input non-maximal ribbonless graph. This algorithm has been implemented here in **ggm** as illustrated below.

Function for generating maximal graphs. Given a non-maximal graph, we can obtain the adjacency matrix of a maximal graph that induces the same independence statements with the function Max. This function uses the algorithm by Sadeghi (2011), which is an extension of the implicit algorithm presented in Richardson and Spirtes (2002). The related functions MAG, MSG, and MRG, are just handy wrappers to obtain maximal AGs, SGs and AGs, respectively. For example,

> plotGraph(H)

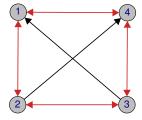


is a mixed non-maximal graph, with the missing edge between nodes 1 and 4 that is not associated with any independence statement. Its associated maximal graph is obtained by

> Max(H)

```
1 2 3 4
1 0 100 0 100
2 100 0 100 1
3 1 100 0 100
4 100 0 100 0
```

> plotGraph(Max(H))



As the graph H is an ancestral graph (as may be verified by the function isAG), we obtain the same result with

> MAG(H)

6 Verifying Markov equivalence

Two graphical models are said to be Markov equivalent when their associated graphs, although nonidentical, imply the same independence structure, that is the same set of independence statements. Thus two Markov equivalent models cannot be discriminated on the basis of statistical tests of independence, even for arbitrary large samples. For instance, the two directed acyclic graphs models $X \leftarrow U \longrightarrow Y$ and $X \leftarrow U \leftarrow Y$ both imply the same single independence statement between X and Y conditionally on U.

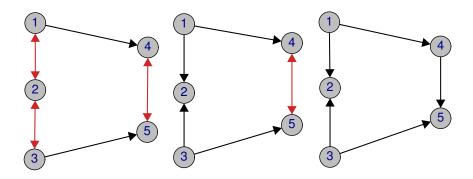
Sometimes, we can check whether graphs of different types are Markov equivalent. For instance the DAG $X \longrightarrow U \longleftarrow Y$ is Markov equivalent to the bi-directed graph $X \longleftrightarrow Z$.

Markov equivalent models may be useful in applications because (a) the may suggest alternative interpretations of a given well-fitting model or (b) on the basis of the equivalence one can choose a simpler fitting algorithm. For instance, the previous bi-directed graph model may be fitted, using the Markov equivalent DAG, in terms of a sequence of univariate regressions.

In the literature several problems related to Markov equivalences have been discussed. These include (a) verifying the Markov equivalence of given graphs, (b) presenting conditions under which a graph of a specific type can be Markov equivalent to a graph of another type, and (c) providing algorithms for generating Markov equivalent graphs of a certain type from a given graph.

Functions for testing Markov equivalences. The function MarkEqRcg tests whether two regression chain graphs are Markov equivalent. This function simply finds the skeleton and all unshielded collider V-configurations in both graphs and tests whether they are identical, see Wermuth and Sadeghi (2012). The arguments of this function are the two graphs a and b in one of the allowed forms. For example,

> plotGraph(H1); plotGraph(H2); plotGraph(H3)

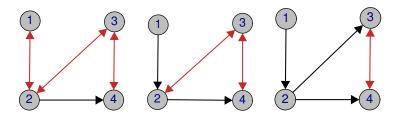


We can now verify Markov equivalence as follows

- > MarkEqRcg(H1,H2)
- [1] TRUE
- > MarkEqRcg(H1,H3)
- [1] FALSE
- > MarkEqRcg(H2,H3)
- [1] FALSE

To test Markov equivalence for maximal ancestral graphs the algorithm is computationally much more demanding (see Ali and Richardson (2004)) and, for this purpose, the function MarkEqMag has been provided. Of course, one can use this function for Markov equivalence of regression chain graphs (which are a subclass of MAGs). For example,

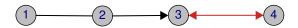
> plotGraph(A1); plotGraph(A2); plotGraph(A3)



- > MarkEqMag(H1,H2)
- [1] TRUE
- > MarkEqMag(H1,H3)
- [1] FALSE
- > MarkEqMag(H2,H3)
- [1] FALSE

Functions for generating Markov equivalent graphs of a specific type. Sometimes is important to verify if a given graph is capable of being Markov equivalent to a graph of a specific class of graphs (such as DAGs, undirected graphs, or bidirected graphs), and if so, to obtain as a result such a graph. The functions RepMarDAG, RepMarUG, and RepMarBG do this for DAGs, undirected graphs, or bidirected graphs, respectively. For associated conditions and algorithms, see Sadeghi (2011). For example, given the following graph

> plotGraph(H)



we can see that it is Markov equivalent to a DAG, by

> RepMarDAG(H)

\$verify

[1] TRUE

\$amat

1 2 3 4

1 0 1 0 0

2 0 0 1 0

3 0 0 0 0

4 0 0 1 0

> plotGraph(RepMarDAG(H))



On the other hand it is not Markov equivalent to an undirected graph or to a bidirected graph.

> RepMarUG(H)

\$verify

[1] FALSE

\$amat

[1] NA

> RepMarBG(H)

\$verify

[1] FALSE

\$amat

[1] NA

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