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The mimR Package for Graphical Modelling in R

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Abstract

The **mimR** package for graphical modelling in R is introduced. We present some facilities of **mimR**, namely those relating specifying models, editing models, fitting models and doing model search. We also discuss the entities needed for flexible graphical modelling in terms of an object structure. An example about a latent variable model is presented.

Keywords: graphical model, mixed interaction model, statistical computing, latent variable model.

1. Introduction and background

The $\min \mathbf{R}^1$ package provides facilities for graphical modelling in the statistical program R (R Development Core Team 2004) and is a part of the gR-project² which is a project to make graphical models available in R. mimR is available as an R-package on the Comprehensive R Archive Network (CRAN)³.

The statistical foundation for **mimR** is Mixed Interaction Models, a very general class of statistical models for mixed discrete and continuous variables. Statistical inference in mixed interaction models can be made with the stand-alone program \mathbf{MIM}^4 , and the core of **mimR** is an interface from R to the **MIM** program. Edwards (2000) describes the models and the **MIM** program in a very clear way. For a comprehensive account of graphical models we refer to Lauritzen (1996). Other important references are Edwards (1990) and Lauritzen and Wermuth (1989). In this paper, the statistical theory behind mixed interaction models will not be outlined; instead the reader is referred to Edwards (2000).

¹http://www.jbs.agrsci.dk/~sorenh/mimR

²http://www.R-project.org/gR

³http://www.R-project.org

⁴available from http://www.hypergraph.dk

2. Preliminaries

2.1. Getting help

In addition to the documentation in the **mimR** package, the **MIM** program itself contains a comprehensive help function which the user of **mimR** is encouraged to make use of.⁵

2.2. Availability

mimR is available only on Windows platforms because MIM only runs on Windows platforms.

2.3. MIM as inference engine

From the users perspective, the **MIM** stand-alone program can be regarded as an "inference engine" which the user (at least in principle) needs not be concerned with. However, in practice it is worth keeping in mind that **MIM** is indeed a stand-alone program rather than integrated with **mimR**: In **MIM** there can at any time be only 1) one specification of a data set, 2) one data set and 3) one model. This means that when fitting a new model, a lot of information may have to be conveyed to **MIM**, and this may take some time (if the data set is large). Likewise, returning fitted values etc. from **MIM** to R may take some time too.

2.4. Installation

Because mimR uses MIM as inference engine, the MIM program must be installed on the computer. The communication between R and MIM is based on the RDCOMClient package. This package, which is not on CRAN, can be downloaded from http://www.omegahat.org/RDCOMClient/. To install the package, download the binary version of the package. Then install the package in R e.g. by choosing Install package(s) from local zip files... in the Packages menu of the RGui.

After completing these installation steps, **mimR** is loaded by the command:

> library(mimR)

2.5. Known problems

When **mimR** invokes **MIM** it sometimes happens that a window with the text Access violation at adrress... pops up. We have not yet been able to track down the source of this error message, but it turns out that **mimR** (and **MIM**) work despite this message. One can often avoid this problem by starting **MIM** manually before starting to use **mimR**.

3. The rats dataset

Some features of **mimR** will be illustrated in the present paper on the basis of the **rats** dataset in the **mimR** package. The **rats** dataset is from a hypothetical drug trial, where the weight

 $^{^5\}mathrm{To}$ access the help function in **MIM** go to the **MIM** program and press F1.

losses of male and female rats under three different drug treatments have been measured after one and two weeks. See Edwards (2000) for more details. To load the data, type

> data(rats)

The first 8 rows of the data are:

> rats[1:8,]

Sex Drug W1 W2 М D1 5 6 1 2 D1 7 М 6 3 9 М D1 9 4 М D1 5 4 D2 9 12 5 М 6 D2 7 7 М 7 7 М D2 6 8 М D2 6 8

4. Objects in mimR

The core of **mimR** are the gmData and mim objects. Informally, a gmData object can be regarded as the **mimR** analogue to a dataframe in R, whereas a mim object can be regarded as the **mimR** analogue to model objects in R, e.g. lm and glm objects. However, there are important exceptions to these analogies:

- gmData objects A gmData object contains information about variables, their labels, their levels (for discrete variables) etc. A gmData object may also contain data, but need not do so. The name "gmData" is short for "graphical meta data". The idea behind separating the specification of the variables from data is that some properties of a model can be investigated without any reference to data, for example decomposability and collapsibility. See Section 5 for details.
- mim objects A mim object links a model formula to a gmData object. Since a gmData object need not contain any data, fitting a mim model is separate process. (This is an important difference between models in mimR and e.g. the lm() function R, which also fits the model to data.) When the model has been fitted (provided that there are data in the gmData object), the mim object also contains the fitted values, parameter estimates etc. See Section 6 for details.

5. gmData objects – graphical meta data

5.1. Making a gmData object from a data frame or a table

Typically one will create a gmData object (with data) from a data frame (or a table) as using the as.gmData() function as follows:

```
> data(rats)
> gmdRats <- as.gmData(rats)</pre>
> gmdRats
  name letter factor levels
                TRUE
1 Sex
            а
                           2
2 Drug
            b
                TRUE
                           3
            c FALSE
                          NA
3
    W1
            d FALSE
4
    W2
                          NA
Data origin:
                   data.frame
To see the values of the factors use the 'vallabels' function
To see the data use the 'observations' function
> data(HairEyeColor)
> gmdHec <- as.gmData(HairEyeColor)</pre>
> gmdHec
  name letter factor levels
                TRUE
1 Hair
            а
                           Δ
                           4
2 Eye
            b
                TRUE
                TRUE
3 Sex
                           2
            с
Data origin:
                   table
To see the values of the factors use the 'vallabels' function
To see the data use the 'observations' function
```

To each variable, there is associated a letter. This letter is used in connection with the internal representation of models and variables in **MIM** and the user should not be concerned with this. It is possible use the letters in specifying models but it is not recommended.

5.2. Creating a gmData object without data

A gmData object (without data) can be created by the gmData() function:

```
> gmdRatsNodata <- gmData(c("Sex", "Drug", "W1", "W2"),</pre>
     factor = c(2, 3, FALSE, FALSE), vallabels = list(c("M", "F")),
     c("D1", "D2", "D3")))
> gmdRatsNodata
  name letter factor levels
1 Sex
            а
                TRUE
                           2
                TRUE
2 Drug
                           3
            b
3
    W1
            c FALSE
                          ΝA
    W2
            d FALSE
4
                          NA
Data origin:
                  table
To see the values of the factors use the 'vallabels' function
To see the data use the 'observations' function
```

```
4
```

With such a specification, one can afterwards specify models and have **mimR** to find important properties of these models, e.g. whether a given model is decomposable.

6. Models in mimR

Currently, only undirected models are available in **mimR**. That is, models in which all variables are treated on equal footing as response variables. (Thus models where a possible response structure has to be accounted for can not be dealt with in **mimR**).

An undirected model is created using the mim() function (which returns a mim object):

```
> mRats <- mim("Sex:Drug/Sex:Drug:W1+Sex:Drug:W2/W1:W2", data = gmdRats)
```

It is possible to specify 1) the main effects, 2) the saturated and 3) the homogeneous saturated models (possibly for only a subset of the variables) in short form:

```
> mainRats <- mim(".", data = gmdRats, marginal = c("Sex", "Drug", "W1"))
> satRats <- mim("..", data = gmdRats, marginal = c("Sex", "Drug", "W1"))
> hsatRats <- mim("..h", data = gmdRats, marginal = c("Sex", "Drug", "W1"))</pre>
```

7. Model fitting

Model fitting is separated from model specification so the models created above are not fitted to data. For model fitting two functions are available: fit() and emfit() (emfit() will be discussed in Section 12).

> mRatsFit <- fit(mRats)</pre>

Deviance: 27.8073 DF: 15

> mRatsFit

Formula: Sex:Drug/Sex:Drug:W1+Sex:Drug:W2/W1:W2
likelihood: 273.705 DF: 15

8. Fitted values (parameter estimates)

The fitted values (parameters estimates) can be obtained using the fitted() function:

```
> fitted(mRatsFit)
```

	Drug	Sex	Freq	W1	W2	W1:W1	W1:W2	W2:W1	W2:W2
1	1	1	4	7.50	8.25	3.938	3.187	3.187	4.75
2	2	1	4	7.75	8.75	3.938	3.187	3.187	4.75
3	3	1	4	13.50	8.50	3.938	3.187	3.187	4.75
4	1	2	4	6.50	6.25	3.938	3.187	3.187	4.75
5	2	2	4	7.25	8.25	3.938	3.187	3.187	4.75
6	3	2	4	16.00	12.00	3.938	3.187	3.187	4.75

The data frame contains for each configuration of the discrete variables 1) the number of cases with that configuration and 2) the estimated mean vector and covariance matrix. The function modelInfo() provides fitted values (along with other information) in a different form.

9. Model summary

A summary (including certain model properties) of a mim can be achieved using the summary() and properties() functions:

```
> summary(mRatsFit)
```

```
Formula: Sex:Drug/Sex:Drug:W1+Sex:Drug:W2/W1:W2
Formula(letter): ab/abc,abd/cd
Variable type: mixed
deviance: 27.8073 DF: 15 likelihood: 273.705
Cliques: [1] "Sex:Drug:W1:W2"
For model properties, use : 'properties()'
For fitting information etc. use : 'modelInfo()'
```

The formula as letters show the internal representation of the models in **MIM**. The variable type being **mixed** shows that the model contains both discrete and continuous variables.

```
> properties(mRatsFit)
```

Variables in model : Sex Drug W1 W2 Is fitted : TRUE Is graphical : TRUE Is decomposable: TRUE Is mean linear : TRUE Is homogeneous : TRUE Is delta-collapsible: TRUE

The model summary reads as follows: 1) The model is fitted to data. 2) The model is graphical (such that there is a 1–1 correspondence between the model and its interaction graph). 3) The model is decomposable meaning that the maximum likelihood estimate exists in closed form (i.e. no iteration is needed). 4) The model is mean linear meaning that the regressions of each continuous variable on the discrete variables all have the same structural form. 5) The model is homogeneous meaning that the variance of the continuous variables does not vary with the levels of the discrete variables. 6) Finally, the model is Δ -collapsible which means that the model can be collapsed onto the discrete variables.

10. Model editing and model selection

10.1. Editing models directly

Models can be edited using the editmim() function by which one can 1) delete edges, 2) add edges, 3) homogeneously add edges, 4) delete terms (interactions) and 5) add terms (see

Edwards (2000) for the precise definitions of these terms). It should be noted that operations are conducted in the order specified above. For example:

```
> mainRats <- mim(".", data = gmdRats)
> m2Rats <- editmim(mainRats, addEdge = c("Sex:Drug", "Sex:W2"))</pre>
```

The model specified this way is heterogeneous as the variance of W2 depends on Sex. Some properties of this model are

```
> summary(m2Rats)
```

```
Formula: Sex:Drug/W1+Sex:W2/W1+Sex:W2
Formula(letter): ab/c,ad/c,ad
Variable type: mixed
Cliques: [1] "Sex:Drug" "Sex:W2" "W1"
For model properties, use : 'properties()'
For fitting information etc. use : 'modelInfo()'
```

> properties(m2Rats)

Variables in model	:	Sex Drug W1 W2
Is fitted	:	FALSE
Is graphical	:	TRUE Is decomposable: TRUE
Is mean linear	:	TRUE Is homogeneous : FALSE
Is delta-collapsible	e:	TRUE

We see that m2Rats is not homogeneous (because the variance of W2 depends on Sex). To add homogeneous terms, the haddEdge keyword can be used as in

```
> m3Rats <- editmim(mainRats, addEdge = "Sex:Drug", haddEdge = "Drug:W1:W2")</pre>
> summary(m3Rats)
Formula: Sex:Drug/Drug:W2+Drug:W1/W1:W2
Formula(letter): ab/bd,bc/cd
Variable type: mixed
 Cliques: [1] "Sex:Drug"
                         "Drug:W1:W2"
For model properties, use : 'properties()'
For fitting information etc. use : 'modelInfo()'
> properties(m3Rats)
 Variables in model : Sex Drug W2 W1
 Is fitted : FALSE
 Is graphical
                   : TRUE
                             Is decomposable: TRUE
 Is mean linear : TRUE
                             Is homogeneous : TRUE
 Is delta-collapsible: TRUE
```

Note the difference between deleting edges and terms:

```
> msatHec <- mim("..", data = gmdHec)
> msatHec
Formula: Hair:Eye:Sex//
> editmim(msatHec, deleteEdge = "Hair:Eye:Sex")
Formula: Sex+Eye+Hair//
> editmim(msatHec, deleteTerm = "Hair:Eye:Sex")
Formula: Eye:Sex+Hair:Sex+Hair:Eye//
```

10.2. Stepwise model selection

To a mim object the function stepwise() applies and this function takes as additional arguments all arguments that the STEPWISE command in MIM does. The stepwise() function returns a new mim object.

```
> data(carcass)
> gmdCarc <- as.gmData(carcass)
> mainCarc <- mim(".", data = gmdCarc)
> satCarc <- mim("..", data = gmdCarc)
> carcForw <- stepwise(mainCarc, arg = "f")
> carcBack <- stepwise(satCarc, arg = "s")</pre>
```

The arg="f" specifies forward selection (default is backward) and arg="s" requests exact tests. The selected models are:

> carcForw

Formula: //F11:F12:M12:F13+F11:F12:M13+F11:F12:M13:LMP+M11:M12:M13 likelihood: 11405.13 DF: 7

> carcBack

```
Formula: //F11:M11:F12:M12:M13+F11:M11:F12:F13:LMP+F11:M11:F12:M13:LMP likelihood: 11370.74 DF: 3
```

11. Missing values and/or latent variables

To fit a model with to incomplete data or to fit a latent variable model, the emfit() function can be used. This function be illustrated in connection with a latent variable model.

12. Example – Mathematics marks

This dataset (taken from Mardia, Kent, and Bibby (1979)) contains the examination marks for 88 students in 5 different subjects. Data is contained the data set mathmark in the mimR package. Edwards (2000) also investigates these data.

12.1. Selecting a graphical model

We start out by specifying the saturated model and do a backward elimination:

```
> data(mathmark)
> gmdMath <- as.gmData(mathmark)
> satMath <- mim("..", data = gmdMath)
> m2Math <- stepwise(satMath)</pre>
```

```
> m2Math
```

```
Formula: //mechanics:vectors:algebra+algebra:analysis:statistics likelihood: 3391.021 DF: 4
```

The model math2 is shown in Figure 1.

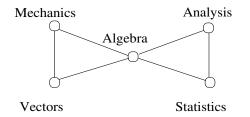


Figure 1: The "butterfly" model selected for the mathmarks data.

12.2. Fitting a model with a discrete latent variable

Next we consider a latent variable model: We suppose that there is a latent binary variable A such that the manifest variables are all conditionally independent given A. We fit such a model by:

```
> math <- mathmark
> math$A <- factor(NA, levels = 1:2)
> gmdMath <- as.gmData(math)</pre>
```

With the specification above, A is a binary variable consisting of NA values. Next, we make explicit in the gmData object that A is indeed a latent variable using the latent() function:

> latent(gmdMath) <- "A"</pre>

In Section 12.4 it will become clear why it must be specified explicitly that A is indeed a latent variable.

One consequence of this last specification is that the model can not be fitted using the fit() function. Instead, the emfit() function which uses the EM algorithm Dempster, Laird, and Rubin (1977), must be used:

```
> satMath <- mim("..", data = gmdMath)
> mathNames <- names(mathmark)
> mathNames
[1] "mechanics" "vectors" "algebra" "analysis"
[5] "statistics"
> delEdges <- paste(mathNames, collapse = ":")
> delEdges
[1] "mechanics:vectors:algebra:analysis:statistics"
> m2Math <- editmim(satMath, deleteEdge = delEdges)</pre>
```

```
> m2MathFit <- emfit(m2Math, plot = TRUE)</pre>
```

The argument plot=TRUE in emfit() creates the plot in Figure 2.

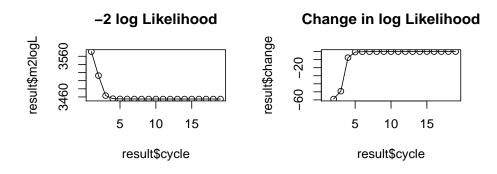


Figure 2: Convergence of the EM algorithm.

On the basis of the fitted model, **mimR** can impute the latent variables. For discrete latent variables this amounts for each case to assign the value with the highest probability. For a continuous latent variable, the imputed values is the conditional mean of the latent variable given the observed variables. To impute the missing values we use the **imputeMissing()** function (which takes no arguments) as:

> imputeMissing()

To get the data (including the imputed values) we use the **retrieveData()** function (which takes no arguments):

```
> d.imp <- retrieveData()</pre>
> d.imp[1:5, ]
  mechanics vectors algebra analysis statistics A
          77
                    82
                             67
                                        67
                                                     81 2
1
2
          63
                    78
                             80
                                        70
                                                     81 2
3
          75
                    73
                             71
                                        66
                                                     81 2
4
          55
                    72
                             63
                                        70
                                                     68 2
5
          63
                    63
                             65
                                        70
                                                     63 2
```

and so we see that the first 5 cases are assignes A to have level 1.

Next, we plot the predicted value of A against the observation number:

> plot(d.imp\$A)

The plot is shown in Figure 3. The grouping of the values of A suggests that data have been processed somehow prior to presentation. Edwards (2000), p. 181, conclude: "Certainly they (the data) have been mistreated in some way, doubtless by a statistician."

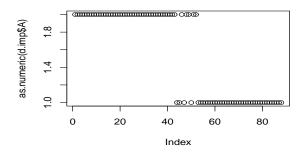


Figure 3: An index plot of the discrete latent variable A.

12.3. Controlling the EM algorithm

The EM algorithm needs a set of initial values for the unobserved values to start from when calculating the parameter estimates in the first iteration. It is well known, that the final estimate of the EM algorithm may depend on the initial values and that (especially in the case of latent variables) the likelihood may have multiple maxima. Default in the call of emfit() is that **MIM** substitutes random values for the missing values. It is, however, possible to control the starting values of the EM algorithm as follows: The user can 1) specify the values of **A** and 2) subsequently declare **A** to be latent. In the call of emfit(), the argument **S** causes the EM algorithm to take the specified values as starting point for the EM algorithm.

12.4. Fitting a model with a continuous latent variable

To illustrate controlling of the EM algorithm, we make an alternative analysis, where A is regarded as a continuous variable. To speed up the convergence of the EM algorithm, we do a factor analysis to get good starting values:

```
> fa <- factanal(mathmark, factors = 1, scores = "regression")
> math$A <- fa$scores</pre>
```

Then we create a gmData object with this new augmented data set and declares that A is to be regarded as a latent variable:

```
> gmdMath <- as.gmData(math)
> latent(gmdMath) <- "A"
> satMath <- mim("..", data = gmdMath)
> m2Math <- editmim(satMath, deleteEdge = delEdges)
> m2MathFit <- emfit(m2Math, arg = "S")</pre>
```

As before we impute the missing values, retrieve the data to R and plot the imputed values for the latent variable:

> imputeMissing()
> d.imp <- retrieveData()
> plot(d.imp\$A)

The plot of the imputed values for the latent variables are shown in Figure 4 and this also suggests that the data do not emerge in random order.

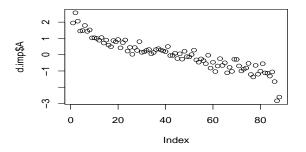


Figure 4: An index of the predicted value of the continuous latent variable A.

13. Discussion

In this paper we have illustrated some aspects of the **mimR** package for graphical modelling in R. It is the hope that **mimR** will be obsolete in a not too distant future – not because of lack of relevance of being able to work with graphical models in R. Rather, it is the hope that a more proper package with with at least the functionality of **mimR** will be created. That is one of the aims of the gR-project, which has lead to the minimal package gRbase which is available on CRAN. The functionality of gRbase is however very limited and as such **mimR** is a relevant package to use for graphical modelling in R.

14. Acknowledgements

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