On the usage of the \texttt{gRim} package

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1 Introduction

The gRim package is an R package for graphRical interaction models (hence the name). gRim implements 1) graphical log-linear models for discrete data, that is for contingency tables and 2) Gaussian graphical models for continuous data (multivariate normal data) and 3) mixed homogeneous interaction models for mixed data (data consisting of both discrete and continuous variables).

The package is at an early stage of development and so is this document.

2 Introductory examples

The main functions for creating models of the various types are:

- Discrete data: The \texttt{dmod()} function creates a hierarchical log-linear model.
- Continuous data: The \texttt{cmod()} function creates a Gaussian graphical model.
- Mixed data: The \texttt{mmod()} function creates a mixed interaction model.

The arguments to the model functions are:

\begin{verbatim}
> args(dmod)
function (formula, data, marginal = NULL, interactions = NULL,
     fit = TRUE, details = 0, ...)
NULL
> args(cmod)
function (formula, data, marginal = NULL, fit = TRUE, details = 0)
NULL
> args(mmod)
function (formula, data, marginal = NULL, fit = TRUE, details = 0)
NULL
\end{verbatim}

The model objects created by these functions are of the respective classes \texttt{dModel}, \texttt{cModel} and \texttt{mModel}. All models are also of the class \texttt{iModel}. We focus the presentation on models for discrete data, but most of the topics we discuss apply to all types of models.

2.1 A Discrete Model

The \texttt{reinis} data from \texttt{gRbase} is a $2^6$ contingency table.
Models are specified as generating classes. A generating class can be a list or a right-hand-sided formula. In addition, various model specification shortcuts are available. Some of these are described in Section 2.2.

The following two specifications of a log-linear model are equivalent:

```r
> data(reinis)
> dm1 <- dmod(list(c("smoke","systol"),c("smoke","mental","phys")), data=reinis)
> dm1 <- dmod(~smoke:systol + smoke:mental:phys, data=reinis)
> dm1

Model: A dModel with 4 variables

-2logL : 9391.38 mdim : 9 aic : 9409.38
ideviance : 730.47 idf : 5 bic : 9459.05
deviance : 3.80 df : 6
```

The output reads as follows: -2logL is minus twice the maximized log-likelihood and mdim is the number of parameters in the model (no adjustments have been made for sparsity of data). The ideviance and idf gives the deviance and degrees of freedom between the model and the independence model for the same variables and deviance and df is the deviance and degrees of freedom between the model and the saturated model for the same variables.

Section 8.1 describes model objects in more detail. Here we just notice that the generating class of the model is contained in the slot glist:

Notice that the generating class does not appear directly. However the generating class can be retrieved using `formula()` and `terms()`.
> formula(dm1)

~smoke * mental * phys + smoke * systol

> str(terms(dm1))

List of 2
$ : chr [1:3] "smoke" "mental" "phys"
$ : chr [1:2] "smoke" "systol"

A summary of a model is provided by the `summary()` function:

```r
> summary(dm1)

             Length Class Mode
modelinfo    3  -none-  list
varNames     4  -none- character
datainfo     1  -none-  list
fitinfo      9  -none-  list
isFitted     1  -none- logical
.call        3  -none-  call
```

### 2.2 Model specification shortcuts

Below we illustrate various other ways of specifying log–linear models.

- A saturated model can be specified using `~.^`. whereas `~.^2` specifies the model with all–two–factor interactions. Using `~.^1` specifies the independence model.

- If we want, say, at most two–factor interactions in the model we can use the `interactions` argument.

- Attention can be restricted to a subset of the variables using the `marginal` argument.

- Variable names can be abbreviated.

The following models illustrate these abbreviations:

---

1 The summary() method leaves a bit to be desired...


```r
> dm2 <- dmod(~.^2, margin=c("smo","men","phy","sys"),
+     data=reinis)
> formula(dm2)

~smoke * mental + smoke * phys + smoke * systol + mental * phys +
   mental * systol + phys * systol

> dm3 <- dmod(list(c("smoke", "systol"), c("smoke", "mental", "phys")),
+     data=reinis, interactions=2)
> formula(dm3)

~smoke * mental + smoke * phys + mental * phys + smoke * systol
```

### 2.3 Plotting models

There are two methods for plotting the dependence graph of a model: Using `iplot()` and `plot()`. The convention for both methods is that discrete variables are drawn as grey dots and continuous variables as white dots.  
1) `iplot()` creates an `igraph` object and plots this.  
2) `plot()` creates a `graphNEL` object and plots this.

```r
> iplot(dm1)
```

![Dependency graph](attachment:dependency_graph.png)

### 2.4 A Continuous Model

For Gaussian models there are at most second order interactions. Hence we may specify the saturated model in different ways:
> data(carcass)
> cm1 <- cmod(~Fat11:Fat12:Fat13, data=carcass)
> cm1 <- cmod(~Fat11:Fat12 + Fat12:Fat13 + Fat11:Fat13, data=carcass)
> cm1

Model: A cModel with 3 variables
-2logL : 4329.16 mdim : 6 aic : 4341.16
ideviance : 886.10 idf : 3 bic : 4364.20
deviance : -0.00 df : 0

> iplot(cm1)

2.5 A Mixed Model

> data(milkcomp1)
> mm1 <- mmod(~.^., data=milkcomp1)
> mm1

Model: A mModel with 5 variables
-2logL : 475.92 mdim : 44 aic : 563.92
deviance : 0.00 df : 0

> iplot(mm1)

2 Harmonize cmod() output with that of dmod()
3 Harmonize mmod() output with that of dmod()
3 Model editing - update()

The update() function enables dModel objects to be modified by the addition or deletion of interaction terms or edges, using the arguments aterm, dterm, aedge or dedge. Some examples follow:

- Set a marginal saturated model:

```r
> ms <- dmod(~.^., marginal=c("phys","mental","systol","family"), data=reinis)  
> formula(ms)

~phys * mental * systol * family
```

- Delete one edge:

```r
> ms1 <- update(ms, list(dedge=~phys:mental))  
> formula(ms1)

~phys * systol * family + mental * systol * family
```

- Delete two edges:

```r
> ms2<- update(ms, list(dedge=~phys:mental+systol:family))  
> formula(ms2)

~phys * systol + phys * family + mental * systol + mental * family
```

- Delete all edges in a set:

```r
```
• Delete an interaction term

```r
> ms4 <- update(ms, list(dterm=~phys:mental:systol))
> formula(ms4)
~phys * mental * family + phys * systol * family + mental * systol * family
```

• Add three interaction terms:

```r
> ms5 <- update(ms, list(aerm=~phys:mental+phys:systol+mental:systol))
> formula(ms5)
~phys * mental * systol * family
```

• Add two edges:

```r
> ms6 <- update(ms, list(aedge=~phys:mental+systol:family))
> formula(ms6)
~phys * mental * systol * family
```

A brief explanation of these operations may be helpful. To obtain a hierarchical model when we delete a term from a model, we must delete any higher-order relatives to the term. Similarly, when we add an interaction term we must also add all lower-order relatives that were not already present. Deletion of an edge is equivalent to deleting the corresponding two-factor term. Let \( m - e \) be the result of deleting edge \( e \) from a model \( m \). Then the result of adding \( e \) is defined as the maximal model \( m^* \) for which \( m^* - e = m \).

4 Testing for conditional independence

Tests of general conditional independence hypotheses of the form \( u \perp \perp v \mid W \) can be performed using the `ciTest()` function.
> cit <- ciTest(reinis, set=c("systol","smoke","family","phys"))

Testing systol _⊥⊥_ smoke | family phys
Statistic (DEV): 13.045 df: 4 p-value: 0.0111 method: CHISQ
Slice information:

<table>
<thead>
<tr>
<th>statistic</th>
<th>p.value</th>
<th>df</th>
<th>family</th>
<th>phys</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.734420</td>
<td>0.029565</td>
<td>1</td>
<td>y</td>
<td>y</td>
</tr>
<tr>
<td>0.003456</td>
<td>0.953121</td>
<td>1</td>
<td>n</td>
<td>y</td>
</tr>
<tr>
<td>7.314160</td>
<td>0.006841</td>
<td>1</td>
<td>y</td>
<td>n</td>
</tr>
<tr>
<td>0.993337</td>
<td>0.318928</td>
<td>1</td>
<td>n</td>
<td>n</td>
</tr>
</tbody>
</table>

The general syntax of the set argument is of the form \((u, v, W)\) where \(u\) and \(v\) are variables and \(W\) is a set of variables. The set argument can also be given as a right-hand sided formula.

In model terms, the test performed by ciTest() corresponds to the test for removing the edge \(\{u, v\}\) from the saturated model with variables \(\{u, v\} \cup W\). If we (conceptually) form a factor \(S\) by crossing the factors in \(W\), we see that the test can be formulated as a test of the conditional independence \(u \perp v \mid S\) in a three way table. The deviance decomposes into independent contributions from each stratum:

\[
D = 2 \sum_{i,j,s} n_{ijs} \log \frac{n_{ijs}}{m_{ijs}} = \sum_s 2 \sum_{i,j} n_{ijs} \log \frac{n_{ijs}}{m_{ijs}} = \sum_s D_s
\]

where the contribution \(D_s\) from the \(s\)th slice is the deviance for the independence model of \(u\) and \(v\) in that slice. For example,

> cit$slice

<table>
<thead>
<tr>
<th>statistic</th>
<th>p.value</th>
<th>df</th>
<th>family</th>
<th>phys</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.734420</td>
<td>0.029565</td>
<td>1</td>
<td>y</td>
<td>y</td>
</tr>
<tr>
<td>0.003456</td>
<td>0.953121</td>
<td>1</td>
<td>n</td>
<td>y</td>
</tr>
<tr>
<td>7.314160</td>
<td>0.006841</td>
<td>1</td>
<td>y</td>
<td>n</td>
</tr>
<tr>
<td>0.993337</td>
<td>0.318928</td>
<td>1</td>
<td>n</td>
<td>n</td>
</tr>
</tbody>
</table>

The \(s\)th slice is a \(u \times v\) table \(\{n_{ijs}\}_{i=1..u, j=1..v}\). The number of degrees of freedom corresponding to the test for independence in this slice is

\[
df_s = (\#\{i : n_{i,s} > 0\} - 1)(\#\{j : n_{j,s} > 0\} - 1)
\]

where \(n_{i,s}\) and \(n_{j,s}\) are the marginal totals.

An alternative to the asymptotic \(\chi^2\) test is to determine the reference distribution using Monte Carlo methods. The marginal totals are sufficient statistics under the null hypothesis, and in a conditional test the test statistic is evaluated in the conditional distribution
given the sufficient statistics. Hence one can generate all possible tables with those given margins, calculate the desired test statistic for each of these tables and then see how extreme the observed test statistic is relative to those of the calculated tables. A Monte Carlo approximation to this procedure is to randomly generate large number of tables with the given margins, evaluate the statistic for each simulated table and then see how extreme the observed test statistic is in this distribution. This is called a Monte Carlo exact test and it provides a Monte Carlo p-value:

```r
> ciTest(reinis, set=c("systol","smoke","family","phys"), method='MC')
```

<table>
<thead>
<tr>
<th>Slice information:</th>
<th>statistic</th>
<th>n.extreme</th>
<th>p.value</th>
<th>df</th>
<th>family</th>
<th>phys</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4.734420</td>
<td>48</td>
<td>0.0240</td>
<td>NA</td>
<td>y</td>
<td>y</td>
</tr>
<tr>
<td>2</td>
<td>0.003456</td>
<td>1716</td>
<td>0.8580</td>
<td>NA</td>
<td>n</td>
<td>y</td>
</tr>
<tr>
<td>3</td>
<td>7.314160</td>
<td>15</td>
<td>0.0075</td>
<td>NA</td>
<td>y</td>
<td>n</td>
</tr>
<tr>
<td>4</td>
<td>0.993337</td>
<td>577</td>
<td>0.2885</td>
<td>NA</td>
<td>n</td>
<td>n</td>
</tr>
</tbody>
</table>

## 5 Fundamental methods for inference

This section describes some fundamental methods for inference in gRim. As basis for the description consider the following model shown in Fig. 1:

```r
> dm5 <- dmod(~ment:phys:systol+ment:systol:family+phys:systol:smoke, + data=reinis)
```

Model: A dModel with 5 variables

<table>
<thead>
<tr>
<th></th>
<th>-2logL</th>
<th>mdim</th>
<th>aic</th>
<th>bic</th>
</tr>
</thead>
<tbody>
<tr>
<td>-2logL</td>
<td>10888.82</td>
<td>15</td>
<td>10918.82</td>
<td>11001.59</td>
</tr>
<tr>
<td>ideviance</td>
<td>732.29</td>
<td>10</td>
<td>11001.59</td>
<td></td>
</tr>
</tbody>
</table>
| deviance      | 25.59      | 16   |        |}

### 5.1 Testing for addition and deletion of edges

Let $\mathcal{M}_0$ be a model and let $e = \{u, v\}$ be an edge in $\mathcal{M}_0$. The candidate model formed by deleting $e$ from $\mathcal{M}_0$ is $\mathcal{M}_1$. The `testdelete()` function can be used to test for deletion of an edge from a model:
Figure 1: A decomposable graphical model for the reinis data.

In the first case the $p$–value suggests that the edge can not be deleted. In the second case the $p$–value suggests that the edge can be deleted. The reported AIC value is the difference in AIC between the candidate model and the original model. A negative value of AIC suggest that the candidate model is to be preferred.

Next, let $M_0$ be a model and let $e = \{u, v\}$ be an edge not in $M_0$. The candidate model formed by adding $e$ to $M_0$ is denoted $M_1$. The testadd() function can be used to test for deletion of an edge from a model:

The $p$–value suggests that no significant improvedment of the model is obtained by adding the edge. The reported AIC value is the difference in AIC between the candidate model and the original model. A negative value of AIC would have suggested that the candidate model is to be preferred.
5.2 Finding edges

The `getInEdges()` function will return a list of all the edges in the dependency graph $G$ defined by the model. If we set `type='decomposable'` then the edges returned are as follows: An edge $e = \{u, v\}$ is returned if $G$ minus the edge $e$ is decomposable. In connection with model selection this is convenient because it is thereby possibly to restrict the search to decomposable models.

```r
> ed.in <- getInEdges(ugList(terms(dm5)), type="decomposable")
[,1] [,2]
[1,] "mental" "phys"
[2,] "mental" "family"
[3,] "phys" "smoke"
[4,] "systol" "family"
[5,] "systol" "smoke"
```

The `getOutEdges()` function will return a list of all the edges which are not in the dependency graph $G$ defined by the model. If we set `type='decomposable'` then the edges returned are as follows: An edge $e = \{u, v\}$ is returned if $G$ plus the edge $e$ is decomposable. In connection with model selection this is convenient because it is thereby possibly to restrict the search to decomposable models.

```r
> ed.out <- getOutEdges(ugList(terms(dm5)), type="decomposable")
[,1] [,2]
[1,] "mental" "smoke"
[2,] "phys" "family"
```

\[A\] function for testing addition / deletion of more general terms is needed.
5.3 Testing several edges

> args(testInEdges)

function (object, edgeMAT = NULL, criterion = "aic", k = 2, alpha = NULL, headlong = FALSE, details = 1, ...)

NULL

> args(testOutEdges)

function (object, edgeMAT = NULL, criterion = "aic", k = 2, alpha = NULL, headlong = FALSE, details = 1, ...)

NULL

The functions `labelInEdges()` and `labelOutEdges()` will test for deletion of edges and addition of edges. The default is to use AIC for evaluating each edge. It is possible to specify the penalty parameter for AIC to being other values than 2 and it is possible to base the evaluation on significance tests instead of AIC. Setting `headlong=TRUE` causes the function to exit once an improvement is found. For example:

> testInEdges(dm5, getInEdges(ugList(terms(dm5)), type="decomposable"), k=log(sum(reinis)))

<table>
<thead>
<tr>
<th>statistic</th>
<th>df</th>
<th>p.value</th>
<th>aic</th>
<th>V1</th>
<th>V2</th>
<th>action</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>686.703</td>
<td>2.000e+00</td>
<td>671.667</td>
<td>mental</td>
<td>phys</td>
<td>-</td>
</tr>
<tr>
<td>2</td>
<td>4.693</td>
<td>9.572e-02</td>
<td>-10.344</td>
<td>mental</td>
<td>family</td>
<td>+</td>
</tr>
<tr>
<td>3</td>
<td>28.147</td>
<td>7.726e-07</td>
<td>13.111</td>
<td>phys</td>
<td>smoke</td>
<td>-</td>
</tr>
<tr>
<td>4</td>
<td>1.085</td>
<td>5.813e-01</td>
<td>-13.951</td>
<td>systol</td>
<td>family</td>
<td>+</td>
</tr>
<tr>
<td>5</td>
<td>11.698</td>
<td>2.882e-03</td>
<td>-3.338</td>
<td>systol</td>
<td>smoke</td>
<td>+</td>
</tr>
</tbody>
</table>

6 Stepwise model selection

Two functions are currently available for model selection: `backward()` and `forward()`. These functions employ the functions in Section 5.3)

6.1 Backward search

For example, we start with the saturated model and do a backward search.
Default is to search among decomposable models if the initial model is decomposable. Default is also to label all edges (with AIC values); however setting `search='headlong'` will cause the labelling to stop once an improvement has been found.

### 6.2 Forward search

Forward search works similarly; for example we start from the independence model:
> dm.i <- dmod(~.^1, data=reinis)
> dm.forw <- forward(dm.i)

change.AIC 683.9717 Edge added: mental,phys
change.AIC 25.4810 Edge added: phys,smoke
change.AIC 15.9293 Edge added: mental,protein
change.AIC 10.8092 Edge added: protein,systol
change.AIC 2.7316 Edge added: mental,family
change.AIC 1.9876 Edge added: mental,smoke
change.AIC 16.4004 Edge added: smoke,protein
change.AIC 12.5417 Edge added: smoke,systol

> iplot(dm.forw)

6.3 Fixing edges/terms in model as part of model selection

The stepwise model selection can be controlled by fixing specific edges. For example we can specify edges which are not to be considered in a backward selection:
> fix <- list(c("smoke","phys","systol"), c("systol","protein"))
> fix <- do.call(rbind, unlist(lapply(fix, names2pairs), recursive=FALSE))
> fix

[,1]   [,2]
[1,]  "phys"  "smoke"
[2,]  "smoke"  "systol"
[3,]  "phys"  "systol"
[4,]  "protein"  "systol"

> dm.s3 <- backward(dm.sat, fixin=fix, details=1)

change.AIC  -19.7744  Edge deleted: mental,systol
change.AIC   -4.6982  Edge deleted: systol,family
change.AIC   -6.8301  Edge deleted: protein,family
change.AIC    -1.2294  Edge deleted: mental,protein
change.AIC    -0.9819  Edge deleted: phys,family
change.AIC    -1.3419  Edge deleted: smoke,family

There is an important detail here: The matrix fix specifies a set of edges. Submitting
these in a call to backward does not mean that these edges are forced to be in the model.
It means that those edges in fixin which are in the model will not be removed.
Likewise in forward selection:

> dm.i3 <- forward(dm.i, fixout=fix, details=1)

change.AIC   683.9717  Edge added: mental,phys
change.AIC    15.9293  Edge added: mental,protein
change.AIC    15.4003  Edge added: smoke,protein
change.AIC     8.6638  Edge added: smoke,mental
change.AIC     2.7316  Edge added: mental,family
change.AIC     1.1727  Edge added: phys,protein

Edges in fix will not be added to the model but if they are in the starting model already,
they will remain in the final model.

7 Further topics on models for contingency tables

7.1 Adjusting for sparsity

Comment on adjustment for sparsity in testadd() and testdelete()
7.2 Dimension of a log–linear model

The \texttt{loglinDim()} is a general function for finding the dimension of a log–linear model. It works on the generating class of a model being represented as a list:

\begin{verbatim}
> dim_loglin(terms(dm2), reinis)
[1] 10
\end{verbatim}

8 Miscellaneous

8.1 The Model Object

It is worth looking at the information in the model object:

\begin{verbatim}
> dm3 <- dmod(list(c("smoke", "systol"), c("smoke", "mental", "phys")),
+ data=reinis)
> names(dm3)
[1] "modelinfo" "varNames" "datainfo" "fitinfo" "isFitted" ".call"
\end{verbatim}

• The model, represented as a list of generators, is

\begin{verbatim}
> str(terms(dm3))
List of 2
$ : chr [1:3] "smoke" "mental" "phys"
$ : chr [1:2] "smoke" "systol"
\end{verbatim}

\begin{verbatim}
> str(dm3$glistNUM)
NULL
\end{verbatim}

The numeric representation of the generators refers back to

\begin{verbatim}
> dm3$varNames
[1] "smoke" "mental" "phys" "systol"
\end{verbatim}

Notice the model object does not contain a graph object. Graph objects are generated on the fly when needed.

• Information about the variables etc. is
> str(dm3[c("varNames","conNames","conLevels")])

List of 3
$ varNames: chr [1:4] "smoke" "mental" "phys" "systol"
$ NA : NULL
$ NA : NULL

- Finally `isFitted` is a logical for whether the model is fitted; `data` is the data (as a table) and `fitinfo` consists of fitted values, logL, df etc.