Generalized nonlinear models in R: An overview of the gnm package

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Contents

1   Introduction

The gnm package provides facilities for fitting *generalized nonlinear models*, i.e., regression models in which the link-transformed mean is described as a sum of predictor terms, some of which may be non-linear in the unknown parameters. Linear and generalized linear models, as handled by the `lm` and `glm` functions in R, are included in the class of generalized nonlinear models, as the special case in which there is no nonlinear term.

This document gives an extended overview of the gnm package, with some examples of applications. The primary package documentation in the form of standard help pages, as viewed in R by, for example, `?gnm` or `help(gnm)`, is supplemented rather than replaced by the present document.

We begin below with a preliminary note (Section 2) on some ways in which the gnm package extends R's facilities for specifying, fitting and working with generalized *linear* models. Then (Section 3 onwards) the facilities for nonlinear terms are introduced, explained and exemplified.

The gnm package is installed in the standard way for CRAN packages, for example by using `install.packages`. Once installed, the package is loaded into an R session by

```
> library(gnm)
```

2   Generalized linear models

2.1   Preamble

Central to the facilities provided by the gnm package is the model-fitting function *gnm*, which interprets a model formula and returns a model object. The user interface of *gnm* is patterned after *glm* (which is included in R's standard stats package), and indeed *gnm* can be viewed as a replacement for *glm* for specifying and fitting generalized linear models. In general there is no reason to prefer *gnm* to *glm* for fitting generalized linear models, except perhaps when the model involves a large number of incidental parameters which are treatable by *gnm*'s *eliminate* mechanism (see Section 4.4).

While the main purpose of the gnm package is to extend the class of models to include nonlinear terms, some of the new functions and methods can be used also with the familiar `lm` and `glm` model-fitting functions. These are: three new data-manipulation functions *Diag*, *Symm* and *Topo*, for setting up structured interactions between factors; a new *family* function, *wedderburn*, for modelling a continuous response variable in [0, 1] with the variance function $V(\mu) = \mu^2(1 - \mu)^2$ as in Wedderburn (1974); and a new generic function `termPredictors` which extracts the contribution of each term to the predictor from a fitted model object. These functions are briefly introduced here, before we move on to the main purpose of the package, nonlinear models, in Section 3.

2.2   *Diag* and *Symm*

When dealing with *homologous* factors, that is, categorical variables whose levels are the same, statistical models often involve structured interaction terms which exploit the inherent symmetry. The functions *Diag* and *Symm* facilitate the specification of such structured interactions.

As a simple example of their use, consider the log-linear models of *quasi-independence*, *quasi-symmetry* and *symmetry* for a square contingency table. Agresti (2002), Section 10.4, gives data on migration between regions of the USA between 1980 and 1985:

```
> count <- c(11607,    100,    366,    124,
+               87, 13677,    515,    302,
+              172,   225, 17819,    270,
+               63,   176,    286, 10192 )
> region <- c("NE", "MW", "S", "W")
> row <-  gl(4, 4, labels = region)
> col <-  gl(4, 1, length = 16, labels = region)
```

The comparison of models reported by Agresti can be achieved as follows:

```
> independence <- glm(count ~ row + col, family = poisson)
> quasi.indep <- glm(count ~ row + col + Diag(row, col), family = poisson)
> symmetry <- glm(count ~ Symm(row, col), family = poisson)
> quasi.symm <- glm(count ~ row + col + Symm(row, col), family = poisson)
> comparison1 <- anova(independence, quasi.indep, quasi.symm)
> print(comparison1, digits = 7)

Analysis of Deviance Table

Model 1: count ~ row + col
Model 2: count ~ row + col + Diag(row, col)
Model 3: count ~ row + col + Symm(row, col)
  Resid. Df Resid. Dev Df  Deviance
1         9  125923.29
2         5      69.51  4 125853.78
3         3       2.99  2     66.52

> comparison2 <- anova(symmetry, quasi.symm)
> print(comparison2)

Analysis of Deviance Table

Model 1: count ~ Symm(row, col)
Model 2: count ~ row + col + Symm(row, col)
  Resid. Df Resid. Dev Df Deviance
1         6    243.550
2         3      2.986  3   240.56
```

The `Diag` and `Symm` functions also generalize the notions of diagonal and symmetric interaction to cover situations involving more than two homologous factors.

2.3 *Topo*

More general structured interactions than those provided by `Diag` and `Symm` can be specified using the function `Topo`. (The name of this function is short for 'topological interaction', which is the nomenclature often used in sociology for factor interactions with structure derived from subject-matter theory.)

The `Topo` function operates on any number (k, say) of input factors, and requires an argument named `spec` which must be an array of dimension $L_1 \times \ldots \times L_k$, where L_i is the number of levels for the ith factor. The `spec` argument specifies the interaction level corresponding to every possible combination of the input factors, and the result is a new factor representing the specified interaction.

As an example, consider fitting the 'log-multiplicative layer effects' models described in Xie (1992). The data are 7 by 7 versions of social mobility tables from Erikson et al. (1982):

3

```
> ### Collapse to 7 by 7 table as in Erikson et al. (1982)
> erikson <- as.data.frame(erikson)
> lvl <- levels(erikson$origin)
> levels(erikson$origin) <- levels(erikson$destination) <-
+     c(rep(paste(lvl[1:2], collapse = " + "), 2), lvl[3],
+         rep(paste(lvl[4:5], collapse = " + "), 2), lvl[6:9])
> erikson <- xtabs(Freq ~ origin + destination + country, data = erikson)
```

From sociological theory — for which see Erikson et al. (1982) or Xie (1992) — the log-linear interaction between origin and destination is assumed to have a particular structure:

```
> levelMatrix <- matrix(c(2, 3, 4, 6, 5, 6, 6,
+                         3, 3, 4, 6, 4, 5, 6,
+                         4, 4, 2, 5, 5, 5, 5,
+                         6, 6, 5, 1, 6, 5, 2,
+                         4, 4, 5, 6, 3, 4, 5,
+                         5, 4, 5, 5, 3, 3, 5,
+                         6, 6, 5, 3, 5, 4, 1), 7, 7, byrow = TRUE)
```

The models of table 3 of Xie (1992) can now be fitted as follows:

```
> ## Null association between origin and destination
> nullModel <- gnm(Freq ~ country:origin + country:destination,
+                  family = poisson, data = erikson, verbose = FALSE)
>
> ## Interaction specified by levelMatrix, common to all countries
> commonTopo <- update(nullModel, ~ . +
+                      Topo(origin, destination, spec = levelMatrix),
+                      verbose = FALSE)
>
> ## Interaction specified by levelMatrix, different multiplier for each country
> multTopo <- update(nullModel, ~ . +
+                    Mult(Exp(country), Topo(origin, destination, spec = levelMatrix)),
+                    verbose = FALSE)
>
> ## Interaction specified by levelMatrix, different effects for each country
> separateTopo <- update(nullModel, ~ . +
+                        country:Topo(origin, destination, spec = levelMatrix),
+                        verbose = FALSE)
>
> anova(nullModel, commonTopo, multTopo, separateTopo)

Analysis of Deviance Table

Model 1: Freq ~ country:origin + country:destination
Model 2: Freq ~ Topo(origin, destination, spec = levelMatrix) + country:origin +
    country:destination
Model 3: Freq ~ Mult(country, Topo(origin, destination, spec = levelMatrix)) +
    country:origin + country:destination
Model 4: Freq ~ country:origin + country:destination + country:Topo(origin,
    destination, spec = levelMatrix)
  Resid. Df Resid. Dev  Df Deviance
1       108     4860.0
2       103      244.3   5   4615.7
3       101      216.4   2     28.0
4        93      208.5   8      7.9
```

Here we have used *gnm* to fit all of these log-link models; the first, second and fourth are log-linear and could equally well have been fitted using `glm`.

2.4 The *wedderburn* family

In Wedderburn (1974) it was suggested to represent the mean of a continuous response variable in $[0, 1]$ using a quasi-likelihood model with logit link and the variance function $\mu^2(1 - \mu)^2$. This is not one of the variance functions made available as standard in R's *quasi* family. The *wedderburn* family provides it. As an example, Wedderburn's analysis of data on leaf blotch on barley can be reproduced as follows:

```
> ##  data from Wedderburn (1974), see ?barley
> logitModel <- glm(y ~ site + variety, family = wedderburn, data = barley)
> fit <- fitted(logitModel)
> print(sum((barley$y - fit)^2 / (fit * (1-fit))^2))

[1] 71.17401
```

This agrees with the chi-squared value reported on page 331 of McCullagh and Nelder (1989), which differs slightly from Wedderburn's own reported value.

2.5 *termPredictors*

The generic function *termPredictors* extracts a term-by-term decomposition of the predictor function in a linear, generalized linear or generalized nonlinear model.

As an illustrative example, we can decompose the linear predictor in the above quasi-symmetry model as follows:

```
> print(temp <- termPredictors(quasi.symm))

   (Intercept)       row        col Symm(row, col)
1   -0.2641848 0.0000000 0.000000      9.62354843
2   -0.2641848 0.0000000 4.918310     -0.09198126
3   -0.2641848 0.0000000 1.539852      4.63901793
4   -0.2641848 0.0000000 5.082641      0.00000000
5   -0.2641848 4.8693457 0.000000     -0.09198126
6   -0.2641848 4.8693457 4.918310      0.00000000
7   -0.2641848 4.8693457 1.539852      0.07295506
8   -0.2641848 4.8693457 5.082641     -3.94766844
9   -0.2641848 0.7465235 0.000000      4.63901793
10  -0.2641848 0.7465235 4.918310      0.07295506
11  -0.2641848 0.7465235 1.539852      7.76583039
12  -0.2641848 0.7465235 5.082641      0.00000000
13  -0.2641848 4.4109017 0.000000      0.00000000
14  -0.2641848 4.4109017 4.918310     -3.94766844
15  -0.2641848 4.4109017 1.539852      0.00000000
16  -0.2641848 4.4109017 5.082641      0.00000000

> rowSums(temp) - quasi.symm$linear.predictors

             1             2             3             4             5
 0.000000e+00 -8.881784e-16  0.000000e+00  0.000000e+00 -8.881784e-16
             6             7             8             9            10
 0.000000e+00  0.000000e+00 -8.881784e-16  0.000000e+00  0.000000e+00
            11            12            13            14            15
 1.776357e-15  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00
            16
 0.000000e+00
```

Such a decomposition might be useful, for example, in assessing the relative contributions of different terms or groups of terms.

3 Nonlinear terms

The main purpose of the gnm package is to provide a flexible framework for the specification and estimation of generalized models with nonlinear terms. The facility provided with *gnm* for the specification of nonlinear terms is designed to be compatible with the symbolic language used in *formula* objects. Primarily, nonlinear terms are specified in the model formula as calls to functions of the class *nonlin*. There are a number of *nonlin* functions included in the gnm package. Some of these specify simple mathematical functions of predictors: *Exp*, *Mult*, and *Inv*. Others specify more specialized nonlinear terms, in particular *MultHomog* specifies homogeneous multiplicative interactions and *Dref* specifies diagonal reference terms. Users may also define their own *nonlin* functions.

3.1 Basic mathematical functions of predictors

Most of the *nonlin* functions included in gnm are basic mathematical functions of predictors:

Exp: the exponential of a predictor

Inv: the reciprocal of a predictor

Mult: the product of predictors

Predictors are specified by symbolic expressions that are interpreted as the right-hand side of a *formula* object, except that an intercept is **not** added by default.

The predictors may contain nonlinear terms, allowing more complex functions to be built up. For example, suppose we wanted to specify a logistic predictor with the same form as that used by *SSlogis* (a selfStart model for use with *nls* — see section 6 for more on *gnm* vs. *nls*):

$$\frac{\text{Asym}}{1 + \exp((\text{xmid} - x)/\text{scal})}.$$

This expression could be simplified by re-parameterizing in terms of xmid/scal and 1/scal, however we shall continue with this form for illustration. We could express this predictor symbolically as follows

`~ -1 + Mult(1, Inv(Const(1) + Exp(Mult(1 + offset(-x), Inv(1)))))`

where *Const* is a convenience function to specify a constant in a *nonlin* term, equivalent to *offset(rep(1, nObs))* where *nObs* is the number of observations. However, this is rather convoluted and it may be preferable to define a specialized *nonlin* function in such a case. Section 3.5 explains how users can define custom *nonlin* functions, with a function to specify logistic terms as an example.

One family of models usefully specified with the basic functions is the family of models with multiplicative interactions. For example, the row-column association model

$$\log \mu_{rc} = \alpha_r + \beta_c + \gamma_r \delta_c,$$

also known as the Goodman RC model (Goodman, 1979), would be specified as a log-link model (for response variable *resp*, say), with formula

`resp ~ R + C + Mult(R, C)`

where *R* and *C* are row and column factors respectively. In some contexts, it may be desirable to constrain one or more of the constituent multipliers[1] in a multiplicative interaction to be nonnegative . This may be achieved by specifying the multiplier as an exponential, as in the following 'uniform difference' model (Xie, 1992; Erikson and Goldthorpe, 1992)

$$\log \mu_{rct} = \alpha_{rt} + \beta_{ct} + e^{\gamma_t} \delta_{rc},$$

which would be represented by a formula of the form

`resp ~ R:T + C:T + Mult(Exp(T), R:C)`

---

[1] A note on terminology: the rather cumbersome phrase 'constituent multiplier', or sometimes the abbreviation 'multiplier', will be used throughout this document in preference to the more elegant and standard mathematical term 'factor'. This will avoid possible confusion with the completely different meaning of the word 'factor' — that is, a categorical variable — in R.

3.2 `MultHomog`

`MultHomog` is a *nonlin* function to specify multiplicative interaction terms in which the constituent multipliers are the effects of two or more factors and the effects of these factors are constrained to be equal when the factor levels are equal. The arguments of `MultHomog` are the factors in the interaction, which are assumed to be objects of class *factor*.

As an example, consider the following association model with homogeneous row-column effects:

$$\log \mu_{rc} = \alpha_r + \beta_c + \theta_r I(r = c) + \gamma_r \gamma_c.$$

To fit this model, with response variable named `resp`, say, the formula argument to `gnm` would be

```
resp ~ R + C + Diag(R, C) + MultHomog(R, C)
```

If the factors passed to `MultHomog` do not have exactly the same levels, a common set of levels is obtained by taking the union of the levels of each factor, sorted into increasing order.

3.3 `Dref`

`Dref` is a *nonlin* function to fit diagonal reference terms (Sobel, 1981, 1985) involving two or more factors with a common set of levels. A diagonal reference term comprises an additive component for each factor. The component for factor f is given by

$$w_f \gamma_l$$

for an observation with level l of factor f, where w_f is the weight for factor f and γ_l is the "diagonal effect" for level l.

The weights are constrained to be nonnegative and to sum to one so that a "diagonal effect", say γ_l, is the value of the diagonal reference term for data points with level l across the factors. `Dref` specifies the constraints on the weights by defining them as

$$w_f = \frac{e^{\delta_f}}{\sum_i e^{\delta_i}}$$

where the δ_f are the parameters to be estimated.

Factors defining the diagonal reference term are passed as unspecified arguments to `Dref`. For example, the following diagonal reference model for a contingency table classified by the row factor R and the column factor C,

$$\mu_{rc} = \frac{e^{\delta_1}}{e^{\delta_1} + e^{\delta_2}} \gamma_r + \frac{e^{\delta_2}}{e^{\delta_1} + e^{\delta_2}} \gamma_c,$$

would be specified by a formula of the form

```
resp ~ -1 + Dref(R, C)
```

The `Dref` function has one specified argument, `delta`, which is a formula with no left-hand side, specifying the dependence (if any) of δ_f on covariates. For example, the formula

```
resp ~ -1 + x + Dref(R, C, delta = ~ 1 + x)
```

specifies the generalized diagonal reference model

$$\mu_{rci} = \beta x_i + \frac{e^{\xi_{01} + \xi_{11} x_i}}{e^{\xi_{01} + \xi_{11} x_i} + e^{\xi_{02} + \xi_{12} x_i}} \gamma_r + \frac{e^{\xi_{02} + \xi_{12} x_i}}{e^{\xi_{01} + \xi_{11} x_i} + e^{\xi_{02} + \xi_{12} x_i}} \gamma_c.$$

The default value of `delta` is `~1`, so that constant weights are estimated. The coefficients returned by `gnm` are those that are directly estimated, i.e. the δ_f or the $\xi_{.f}$, rather than the implied weights w_f. However, these weights may be obtained from a fitted model using the `DrefWeights` function, which computes the corresponding standard errors using the delta method.

3.4 `instances`

Multiple instances of a linear term will be aliased with each other, but this is not necessarily the case for nonlinear terms. Indeed, there are certain types of model where adding further instances of a nonlinear term is a natural way to extend the model. For example, Goodman's RC model, introduced in section 3.1

$$\log \mu_{rc} = \alpha_r + \beta_c + \gamma_r \delta_c,$$

is naturally extended to the RC(2) model, with a two-component interaction

$$\log \mu_{rc} = \alpha_r + \beta_c + \gamma_r \delta_c + \theta_r \phi_c.$$

Currently all of the *nonlin* functions in gnm except Dref have an `inst` argument to allow the specification of multiple instances. So the RC(2) model could be specified as follows

`resp ~ R + C + Mult(R, C, inst = 1) + Mult(R, C, inst = 2)`

The convenience function `instances` allows multiple instances of a term to be specified at once

`resp ~ R + C + instances(Mult(R, C), 2)`

The formula is expanded by `gnm`, so that the instances are treated as separate terms. The `instances` function may be used with any function with an `inst` argument.

3.5 Custom *nonlin* functions

3.5.1 General description

Users may write their own *nonlin* functions to specify nonlinear terms which can not (easily) be specified using the *nonlin* functions in the gnm package. A function of class *nonlin* should return a list of arguments for the internal function `nonlinTerms`. The following arguments must be specified in all cases:

`predictors`: a list of symbolic expressions or formulae with no left hand side which represent (possibly nonlinear) predictors that form part of the term.

`term`: a function that takes the arguments `predLabels` and `varLabels`, which are labels generated by `gnm` for the specified predictors and variables (see below), and returns a deparsed mathematical expression of the nonlinear term. Only functions recognised by `deriv` should be used in the expression, e.g. `+` rather than `sum`.

Intercepts are added by default to predictors that are specified by formulae. If predictors are named, these names are used as a prefix for parameter labels or as the parameter label itself in the single-parameter case.

The following arguments of `nonlinTerms` must be specified whenever applicable to the nonlinear term:

`variables`: a list of expressions representing variables in the term (variables with a coefficient of 1).

`common`: a numeric index of `predictors` with duplicated indices identifying single factor predictors for which homologous effects are to be estimated.

The arguments below are optional:

`call`: a call to be used as a prefix for parameter labels.

`match`: (if `call` is non-`NULL`) a numeric index of `predictors` specifying which arguments of `call` the predictors match to — zero indicating no match. If `NULL`, predictors will not be matched to the arguments of `call`.

`start`: a function which takes a named vector of parameters corresponding to the predictors and returns a vector of starting values for those parameters. This function is ignored if the term is nested within another nonlinear term.

Predictors which are matched to a specified argument of `call` should be given the same name as the argument. Matched predictors are labelled using "dot-style" labelling, e.g. the label for the intercept in the first constituent multiplier of the term `Mult(A, B)` would be `"Mult(. + A, 1 + B).(Intercept)"`. It is recommended that matches are specified wherever possible, to ensure parameter labels are well-defined.

The arguments of *nonlin* functions are as suited to the particular term, but will usually include symbolic representations of predictors in the term and/or the names of variables in the term. The function may also have an `inst` argument to allow specification of multiple instances (see 3.4).

3.5.2 Example: a logistic function

As an example, consider writing a *nonlin* function for the logistic term discussed in 3.1:

$$\frac{\text{Asym}}{1 + \exp((\text{xmid} - x)/\text{scal})}.$$

We can consider *Asym*, *xmid* and *scal* as the parameters of three separate predictors, each with a single intercept term. Thus we specify the `predictors` argument to `nonlinTerms` as

```
predictors = list(Asym = 1, xmid = 1, scal = 1)
```

The term also depends on the variable *x*, which would need to be specified by the user. Suppose this is specified to our *nonlin* function through an argument named `x`. Then our *nonlin* function would specify the following `variables` argument

```
variables = list(substitute(x))
```

We need to use `substitute` here to list the variable specified by the user rather than the variable named **"x"** (if it exists).

Our *nonlin* function must also specify the `term` argument to `nonlinTerms`. This is a function that will paste together an expression for the term, given labels for the predictors and the variables:

```
term = function(predLabels, varLabels) {
  paste(predLabels[1], "/(1 + exp((", predLabels[2], "-",
  varLabels[1], ")/", predLabels[3], "))")
}
```

We now have all the necessary ingredients of a *nonlin* function to specify the logistic term. Since the parameterization does not depend on user-specified values, it does not make sense to use call-matched labelling in this case. The labels for our parameters will be taken from the labels of the `predictors` argument. Since we do not anticipate fitting models with multiple logistic terms, our *nonlin* function will not specify a `call` argument with which to prefix the parameter labels. We do however, have some idea of useful starting values, so we will specify the `start` argument as

```
start = function(theta){
    theta[3] <- 1
    theta
}
```

which sets the initial scale parameter to one.

Putting all these ingredients together we have

```
Logistic <- function(x){
    list(predictors = list(Asym = 1, xmid = 1, scal = 1),
         variables = list(substitute(x)),
         term = function(predLabels, varLabels) {
             paste(predLabels[1], "/(1 + exp((", predLabels[2], "-",
             varLabels[1], ")/", predLabels[3], "))")
         },
         start = function(theta){
             theta[3] <- 1
             theta
         })
}
class(Logistic) <- "nonlin"
```

3.5.3 Example: `MultHomog`

The `MultHomog` function included in the gnm package provides a further example of a *nonlin* function, showing how to specify a term with quite different features from the preceding example. The definition is

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```
MultHomog <- function(..., inst = NULL){
    dots <- match.call(expand.dots = FALSE)[["..."]]
    list(predictors = dots,
         common = rep(1, length(dots)),
         term = function(predLabels, ...) {
             paste("(", paste(predLabels, collapse = ")*("), ")", sep = "")},
         call = as.expression(match.call()))
}
class(MultHomog) <- "nonlin"
```

Firstly, the interaction may be based on any number of factors, hence the use of the special "`...`" argument. The use of `match.call` is analogous to the use of `substitute` in the `Logistic` function: to obtain expressions for the factors as specified by the user.

The returned `common` argument specifies that homogeneous effects are to be estimated across all the specified factors. The term only depends on these factors, but the `term` function allows for the empty `varLabels` vector that will be passed to it, by having a "`...`" argument.

Since the user may wish to specify multiple instances, the `call` argument to `nonlinTerms` is specified, so that parameters in different instances of the term will have unique labels (due to the `inst` argument in the call). However as the expressions passed to "`...`" may only represent single factors, rather than general predictors, it is not necessary to use call-matched labelling, so the `match` argument is not specified here.

4   Controlling the fitting procedure

The `gnm` function has a number of arguments which affect the way a model will be fitted. Basic control parameters can be set using the arguments `lsMethod`, `ridge`, `tolerance`, `iterStart` and `iterMax`. Starting values for the parameter estimates can be set by `start` or they can be generated from starting values for the predictors on the link or response scale via `etastart` or `mustart` respectively. Parameters can be constrained via `constrain` and `constrainTo` arguments, while parameters of a stratification factor can be handled more efficiently by specifying the factor in an `eliminate` argument. These options are described in more detail below.

4.1   Basic control parameters

The arguments `iterStart` and `iterMax` control respectively the number of starting iterations (where applicable) and the number of main iterations used by the fitting algorithm. The progress of these iterations can be followed by setting either `verbose` or `trace` to `TRUE`. If `verbose` is `TRUE` and `trace` is `FALSE`, which is the default setting, progress is indicated by printing the character "." at the beginning of each iteration. If `trace` is `TRUE`, the deviance is printed at the beginning of each iteration (over-riding the printing of "." if necessary). Whenever `verbose` is `TRUE`, additional messages indicate each stage of the fitting process and diagnose any errors that cause that cause the algorithm to restart.

Prior to solving the (typically rank-deficient) least squares problem at the heart of the `gnm` fitting algorithm, the design matrix is standardized and regularized (in the Levenberg-Marquardt sense); the `ridge` argument provides a degree of control over the regularization performed (smaller values may sometimes give faster convergence but can lead to numerical instability).

The fitting algorithm will terminate before the number of main iterations has reached `iterMax` if the convergence criteria have been met, with tolerance specified by `tolerance`. Convergence is judged by comparing the squared components of the score vector with corresponding elements of the diagonal of the Fisher information matrix. If, for all components of the score vector, the ratio is less than `tolerance^2`, or the corresponding diagonal element of the Fisher information matrix is less than 1e-20, the algorithm is deemed to have converged.

4.2   Specifying starting values

4.2.1   Using `start`

In some contexts, the default starting values may not be appropriate and the fitting algorithm will fail to converge, or perhaps only converge after a large number of iterations. Alternative starting values may be passed on to `gnm`

by specifying a *start* argument. This should be a numeric vector of length equal to the number of parameters (or possibly the non-eliminated parameters, see Section 4.4), however missing starting values (*NA*s) are allowed.

If there is no user-specified starting value for a parameter, the default value is used. This feature is particularly useful when adding terms to a model, since the estimates from the original model can be used as starting values, as in this example:

```
model1 <- gnm(mu ~ R + C + Mult(R, C))
model2 <- gnm(mu ~ R + C + instances(Mult(R, C), 2),
          start = c(coef(model1), rep(NA, 10)))
```

The *gnm* call can be made with *method = "coefNames"* to identify the parameters of a model prior to estimation, to assist with the specification of arguments such as *start*. For example, to get the number *10* for the value of *start* above, we could have done

```
gnm(mu ~ R + C + instances(Mult(R, C), 2), method = "coefNames")
```

from whose output it would be seen that there are 10 new coefficients in *model2*. When called with *method = "coefNames"*, *gnm* makes no attempt to fit the specified model; instead it returns just the names that the coefficients in the fitted model object would have.

The starting procedure used by *gnm* is as follows:

1. Begin with all parameters set to *NA*.

2. Replace *NA* values with any starting values set by *nonlin* functions.

3. Replace current values with any (non-*NA*) starting values specified by the *start* argument of *gnm*.

4. Set any values specified by the *constrain* argument to the values specified by the *constrainTo* argument (see Section 4.3).

5. Categorise remaining *NA* parameters as linear or nonlinear, treating non-*NA* parameters as fixed. Initialise the nonlinear parameters by generating values θ_i from the Uniform$(-0.1, 0.1)$ distribution and shifting these values away from zero as follows

$$\theta_i = \begin{cases} \theta_i - 0.1 & \text{if } \theta_i < 1 \\ \theta_i + 0.1 & \text{otherwise} \end{cases}$$

6. Compute the *glm* estimate of the linear parameters, offsetting the contribution to the predictor of any terms fully determined by steps 2 to 5.

7. Run starting iterations: update nonlinear parameters one at a time, jointly re-estimating linear parameters after each round of updates.

Note that no starting iterations (step 7) will be run if all parameters are linear, or if all nonlinear parameters are specified by *start*, *constrain* or a *nonlin* function.

4.2.2 Using *etastart* or *mustart*

An alternative way to set starting values for the parameters is to specify starting values for the predictors.

If there are linear parameters in the model, the predictor starting values are first used to fit a model with only the linear terms (offsetting any terms fully specified by starting values given by *start*, *constrain* or a *nonlin* function). In this case the parameters corresponding to the predictor starting values can be computed analytically. If the fitted model reproduces the predictor starting values, then these values contain no further information and they are replaced using the *initialize* function of the specified *family*.

The predictor starting values or their replacement are then used as the response variable in a nonlinear least squares model with only the unspecified nonlinear terms, offsetting the contribution of any other terms. Since the model is over-parameterized, the model is approximated using *iterStart* iterations of the "L-BFGS-B" algorithm of *optim*, assuming parameters lie in the range (-10, 10).

Starting values for the predictors can be specified explicitly via *etastart* or implicitly by passing starting values for the fitted means to *mustart*. For example, when extending a model, the fitted predictors from the first model can be used to find starting values for the parameters of the second model:

```
model1 <- gnm(mu ~ R + C + Mult(R, C))
model2 <- gnm(mu ~ R + C + instances(Mult(R, C), 2), etastart = model1$predictors)
```

Using *etastart* avoids the one-parameter-at-a-time starting iterations, so is quicker than using *start* to pass on information from a nested model. However *start* will generally produce better starting values so should be used when feasible. For multiplicative terms, the *residSVD* functions provides a better way to avoid starting iterations.

4.3 Using *constrain*

By default, *gnm* only imposes identifiability constraints according to the general conventions used by *R* to handle linear aliasing. Therefore models that have any nonlinear terms will be typically be over-parameterized, and *gnm* will return a random parameterization for unidentified coefficients (determined by the randomly chosen starting values for the iterative algorithm, step 5 above).

To illustrate this point, consider the following application of *gnm*, discussed later in Section 7.1:

```
> set.seed(1)
> RChomog1 <- gnm(Freq ~ origin + destination + Diag(origin, destination) +
+                 MultHomog(origin, destination), family = poisson,
+                 data = occupationalStatus, verbose = FALSE)
```

Running the analysis again from a different seed

```
> set.seed(2)
> RChomog2 <- update(RChomog1)
```

gives a different representation of the same model:

```
> compareCoef <- cbind(coef(RChomog1), coef(RChomog2))
> colnames(compareCoef) <- c("RChomog1", "RChomog2")
> round(compareCoef, 4)
```

	RChomog1	RChomog2
(Intercept)	0.2404	0.3058
origin2	0.5101	0.5052
origin3	1.5928	1.5744
origin4	1.8892	1.8577
origin5	0.6692	0.6373
origin6	2.7113	2.6679
origin7	1.3687	1.3159
origin8	1.0974	1.0392
destination2	0.9291	0.9242
destination3	1.9372	1.9188
destination4	2.1776	2.1461
destination5	1.5686	1.5367
destination6	3.0148	2.9714
destination7	2.1203	2.0675
destination8	1.6728	1.6146
Diag(origin, destination)1	1.5267	1.5267
Diag(origin, destination)2	0.4560	0.4560
Diag(origin, destination)3	-0.0160	-0.0160
Diag(origin, destination)4	0.3892	0.3892
Diag(origin, destination)5	0.7385	0.7385
Diag(origin, destination)6	0.1347	0.1347
Diag(origin, destination)7	0.4576	0.4576
Diag(origin, destination)8	0.3885	0.3885
MultHomog(origin, destination)1	-1.4646	1.4421
MultHomog(origin, destination)2	-1.2463	1.2238

```
MultHomog(origin, destination)3  -0.6481   0.6256
MultHomog(origin, destination)4  -0.0642   0.0417
MultHomog(origin, destination)5  -0.0471   0.0246
MultHomog(origin, destination)6   0.4647  -0.4872
MultHomog(origin, destination)7   0.8808  -0.9033
MultHomog(origin, destination)8   1.1244  -1.1469
```

Even though the linear terms are constrained, the parameter estimates for the main effects of *origin* and *destination* still change, because these terms are aliased with the higher order multiplicative interaction, which is unconstrained.

Standard errors are only meaningful for identified parameters and hence the output of *summary.gnm* will show clearly which coefficients are estimable:

```
> summary(RChomog2)

Call:
gnm(formula = Freq ~ origin + destination + Diag(origin, destination) +
    MultHomog(origin, destination), family = poisson, data = occupationalStatus,
    verbose = FALSE)

Deviance Residuals:
       Min         1Q      Median         3Q         Max
-1.659e+00  -4.297e-01  -4.463e-08   3.862e-01   1.721e+00

Coefficients:
                                 Estimate Std. Error z value Pr(>|z|)
(Intercept)                       0.30577         NA      NA       NA
origin2                           0.50522         NA      NA       NA
origin3                           1.57439         NA      NA       NA
origin4                           1.85767         NA      NA       NA
origin5                           0.63728         NA      NA       NA
origin6                           2.66791         NA      NA       NA
origin7                           1.31592         NA      NA       NA
origin8                           1.03921         NA      NA       NA
destination2                      0.92424         NA      NA       NA
destination3                      1.91881         NA      NA       NA
destination4                      2.14611         NA      NA       NA
destination5                      1.53670         NA      NA       NA
destination6                      2.97139         NA      NA       NA
destination7                      2.06751         NA      NA       NA
destination8                      1.61459         NA      NA       NA
Diag(origin, destination)1        1.52667    0.44658   3.419  0.00063
Diag(origin, destination)2        0.45600    0.34595   1.318  0.18747
Diag(origin, destination)3       -0.01598    0.18098  -0.088  0.92965
Diag(origin, destination)4        0.38918    0.12748   3.053  0.00227
Diag(origin, destination)5        0.73852    0.23329   3.166  0.00155
Diag(origin, destination)6        0.13474    0.07934   1.698  0.08945
Diag(origin, destination)7        0.45764    0.15103   3.030  0.00245
Diag(origin, destination)8        0.38847    0.22172   1.752  0.07976
MultHomog(origin, destination)1   1.44208         NA      NA       NA
MultHomog(origin, destination)2   1.22378         NA      NA       NA
MultHomog(origin, destination)3   0.62562         NA      NA       NA
MultHomog(origin, destination)4   0.04174         NA      NA       NA
MultHomog(origin, destination)5   0.02457         NA      NA       NA
MultHomog(origin, destination)6  -0.48719         NA      NA       NA
MultHomog(origin, destination)7  -0.90333         NA      NA       NA
MultHomog(origin, destination)8  -1.14691         NA      NA       NA
```

```
(Dispersion parameter for poisson family taken to be 1)

Std. Error is NA where coefficient has been constrained or is unidentified

Residual deviance: 32.561 on 34 degrees of freedom
AIC: 414.9

Number of iterations: 7
```

Additional constraints may be specified through the `constrain` and `constrainTo` arguments of *gnm*. These arguments specify respectively parameters that are to be constrained in the fitting process and the values to which they should be constrained. Parameters may be specified by a regular expression to match against the parameter names, a numeric vector of indices, a character vector of names, or, if `constrain = "[?]"` they can be selected through a *Tk* dialog. The values to constrain to should be specified by a numeric vector; if `constrainTo` is missing, constrained parameters will be set to zero.

In the case above, constraining one level of the homogeneous multiplicative factor is sufficient to make the parameters of the nonlinear term identifiable, and hence all parameters in the model identifiable. Figure 1 illustrates how the coefficient to be constrained may be specified via a *Tk* dialog, an approach which can be helpful in interactive R sessions.

However for reproducible code, it is best to specify the constrained coefficients directly. For example, the following code specifies that the last level of the homogeneous multiplicative factor should be constrained to zero,

```
> set.seed(1)
> RChomogConstrained1 <- update(RChomog1, constrain = length(coef(RChomog1)))
```

Since all the parameters are now constrained, re-fitting the model will give the same results, regardless of the random seed set beforehand:

```
> set.seed(2)
> RChomogConstrained2 <- update(RChomogConstrained1)
> identical(coef(RChomogConstrained1), coef(RChomogConstrained2))
```

```
[1] FALSE
```

It is not usually so straightforward to constrain all the parameters in a generalized nonlinear model. However use of `constrain` in conjunction with `constrainTo` is usually sufficient to make coefficients of interest identifiable . The functions `checkEstimable` or `getContrasts`, described in Section 5, may be used to check whether particular combinations of parameters are estimable.

4.4 Using `eliminate`

When a model contains the additive effect of a factor which has a large number of levels, the iterative algorithm by which maximum likelihood estimates are computed can usually be accelerated by use of the `eliminate` argument to *gnm*. A factor passed to `eliminate` specifies the first term in the model, replacing any intercept term. So, for example

```
gnm(mu ~ A + B + Mult(A, B), eliminate = strata1:strata2)
```

is equivalent, in terms of the structure of the model, to

```
gnm(mu ~ -1 + strata1:strata2 + A + B + Mult(A, B))
```

However, specifying a factor through `eliminate` has two advantages over the standard specification. First, the structure of the eliminated factor is exploited so that computational speed is improved — substantially so if the number of eliminated parameters is large. Second, eliminated parameters are returned separately from non-eliminated parameters (as an attribute of the `coefficients` component of the returned object). Thus eliminated parameters are excluded from printed model summaries by default and disregarded by *gnm* methods that would not be relevant to such parameters (see Section 5).
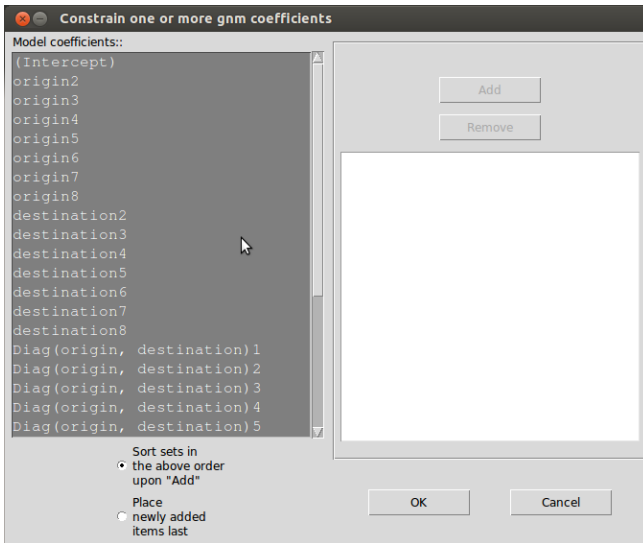
When *gnm* is called with *constrain = "[?]"*, a *Tk* dialog is shown listing the coefficients in the model.
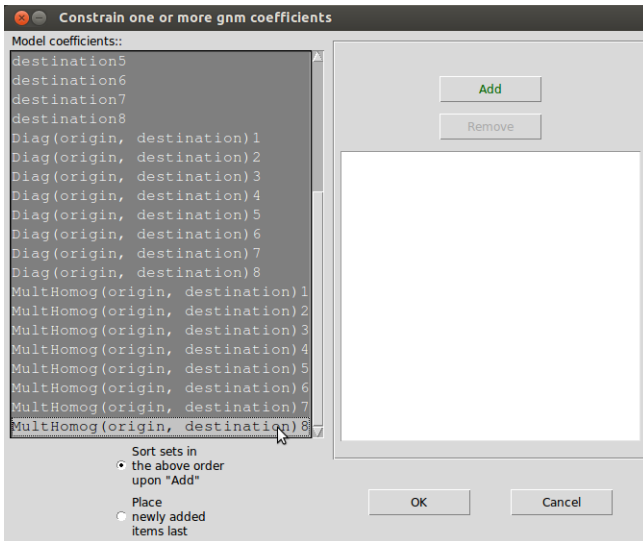
Scroll through the coefficients and click to select a single coefficient to constrain. To select multiple coefficients, hold down the `Ctrl` key whilst clicking. The `Add` button will become active when coefficient(s) have been selected.
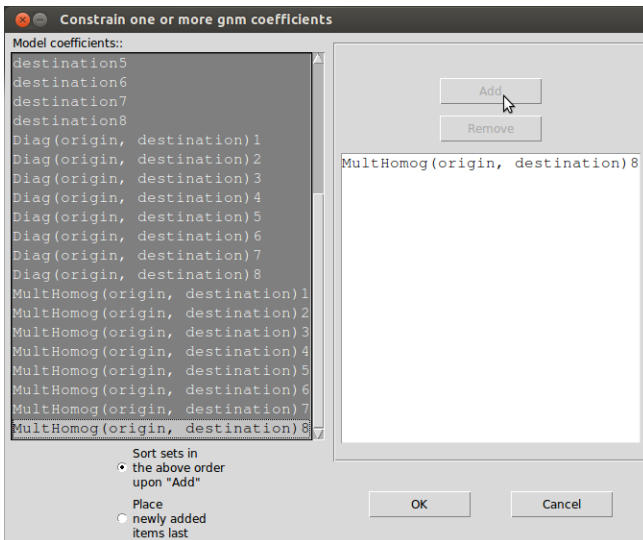
Click the `Add` button to add the selected coefficients to the list of coefficients to be constrained. To remove coefficients from the list, select the coefficients in the right pane and click `Remove`. Click `OK` when you have finalised the list.

Figure 1: Selecting coefficients to constrain with the *Tk* dialog.

The `eliminate` feature is useful, for example, when multinomial-response models are fitted by using the well known equivalence between multinomial and (conditional) Poisson likelihoods. In such situations the sufficient statistic involves a potentially large number of fixed multinomial row totals, and the corresponding parameters are of no substantive interest. For an application see Section 7.6 below. Here we give an artificial illustration: 1000 randomly-generated trinomial responses, and a single predictor variable (whose effect on the data generation is null):

```
> set.seed(1)
> n <- 1000
> x <- rep(rnorm(n), rep(3, n))
> counts <- as.vector(rmultinom(n, 10, c(0.7, 0.1, 0.2)))
> rowID <- gl(n, 3, 3 * n)
> resp <- gl(3, 1, 3 * n)
```

The logistic model for dependence on `x` can be fitted as a Poisson log-linear model[2], using either `glm` or `gnm`:

```
> ## Timings on a Xeon 2.33GHz, under Linux
> system.time(temp.glm <- glm(counts ~ rowID + resp + resp:x,
                                family = poisson))[1]

user.self
   37.126

> system.time(temp.gnm <- gnm(counts ~ resp + resp:x, eliminate = rowID,
                                family = poisson, verbose = FALSE))[1]

user.self
    0.04

> c(deviance(temp.glm), deviance(temp.gnm))

[1] 2462.556 2462.556
```

Here the use of `eliminate` causes the `gnm` calculations to run much more quickly than `glm`. The speed advantage increases with the number of eliminated parameters (here 1000). By default,the eliminated parameters do not appear in printed model summaries as here:

```
> summary(temp.gnm)

Call:

gnm(formula = counts ~ resp + resp:x, eliminate = rowID, family = poisson,
    verbose = FALSE)

Deviance Residuals:
      Min        1Q    Median        3Q       Max
-2.852038 -0.786172 -0.004534  0.645278  2.755013

Coefficients of interest:
        Estimate Std. Error z value Pr(>|z|)
resp2   -1.961448   0.034007 -57.678   <2e-16
resp3   -1.255846   0.025359 -49.523   <2e-16
resp1:x -0.007726   0.024517  -0.315    0.753
resp2:x -0.023340   0.037611  -0.621    0.535
resp3:x  0.000000         NA      NA       NA
```

---

[2]For this particular example, of course, it would be more economical to fit the model directly using `multinom` (from the recommended package nnet). But fitting as here via the 'Poisson trick' allows the model to be elaborated within the gnm framework using `Mult` or other *nonlin* terms.

```
(Dispersion parameter for poisson family taken to be 1)

Std. Error is NA where coefficient has been constrained or is unidentified

Residual deviance: 2462.6 on 1996 degrees of freedom
AIC: 12028

Number of iterations: 4
```

although the `summary` method has a logical `with.eliminate` that can toggled so that the eliminated parameters are included if desired.

The `eliminate` feature as implemented in gnm extends the earlier work of Hatzinger and Francis (2004) to a broader class of models and to over-parameterized model representations.

5 Methods and accessor functions

5.1 Methods

The *gnm* function returns an object of class `c("gnm", "glm", "lm")`. There are several methods that have been written for objects of class *glm* or *lm* to facilitate inspection of fitted models. Out of the generic functions in the base, stats and graphics packages for which methods have been written for *glm* or *lm* objects, Figure 2 shows those that can be used to analyse *gnm* objects, whilst Figure 3 shows those that are not implemented for *gnm* objects.

add1*	family	print
anova	formula	profile
case.names	hatvalues	residuals
coef	labels	rstandard
cooks.distance	logLik	summary
confint	model.frame	variable.names
deviance	model.matrix	vcov
drop1*	plot	weights
extractAIC	predict	

Figure 2: Generic functions in the base, stats and graphics packages that can be used to analyse *gnm* objects. Starred functions are implemented for models with linear terms only.

alias	effects
dfbeta	influence
dfbetas	kappa
dummy.coef	proj

Figure 3: Generic functions in the base, stats and graphics packages for which methods have been written for *glm* or *lm* objects, but which are *not* implemented for *gnm* objects.

In addition to the accessor functions shown in Figure 2, the gnm package provides a new generic function called `termPredictors` that has methods for objects of class *gnm*, *glm* and *lm*. This function returns the additive contribution of each term to the predictor. See Section 2.5 for an example of its use.

Most of the functions listed in Figure 2 can be used as they would be for *glm* or *lm* objects, however care must be taken with `vcov.gnm`, as the variance-covariance matrix will depend on the parameterization of the model. In particular, standard errors calculated using the variance-covariance matrix will only be valid for parameters or contrasts that are estimable!

Similarly, `profile.gnm` and `confint.gnm` are only applicable to estimable parameters. The deviance function of a generalized nonlinear model can sometimes be far from quadratic and `profile.gnm` attempts to detect

assymetry or asymptotic behaviour in order to return a sufficient profile for a given parameter. As an example, consider the following model, described later in Section 7.3:

```
unidiff <- gnm(Freq ~ educ*orig + educ*dest + Mult(Exp(educ), orig:dest),
               constrain = "[.]educ1", family = poisson, data = yaish,
               subset = (dest != 7))
prof <- profile(unidiff, which = 61:65, trace = TRUE)
```

If the deviance is quadratic in a given parameter, the profile trace will be linear. We can plot the profile traces as follows:

Profile traces for the multipliers of the orig:dest association
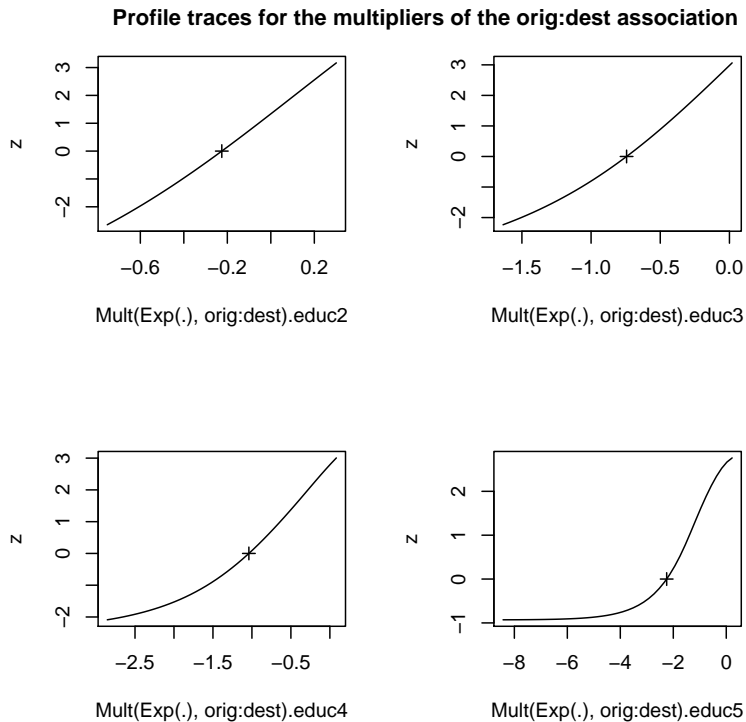
Figure 4: Profile traces for the multipliers of the orig:dest association

From these plots we can see that the deviance is approximately quadratic in `Mult(Exp(.), orig:dest).educ2`, assymetric in `Mult(Exp(.), orig:dest).educ3` and `Mult(Exp(.), orig:dest).educ4` and asymptotic in `Mult(Exp(.), orig:dest).educ5`. When the deviance is approximately quadratic in a given parameter, `profile.gnm` uses the same stepsize for profiling above and below the original estimate:

```
> diff(prof[[2]]$par.vals[, "Mult(Exp(.), orig:dest).educ2"])
```

```
 [1] 0.1053072 0.1053072 0.1053072 0.1053072 0.1053072 0.1053072 0.1053072
 [8] 0.1053072 0.1053072 0.1053072
```

When the deviance is asymmetric, `profile.gnm` uses different step sizes to accommodate the skew:

```
> diff(prof[[4]]$par.vals[, "Mult(Exp(.), orig:dest).educ4"])
```

```
 [1] 0.2018393 0.2018393 0.2018393 0.2018393 0.2018393 0.2018393 0.2018393
 [8] 0.2018393 0.2018393 0.2243673 0.2243673 0.2243673 0.2243673 0.2243673
```

Finally, the presence of an asymptote is recorded in the `"asymptote"` attribute of the returned profile:

```
> attr(prof[[5]], "asymptote")
```

```
[1]  TRUE FALSE
```

This information is used by `confint.gnm` to return infinite limits for confidence intervals, as appropriate:

```
> confint(prof, level = 0.95)
```

```
                                    2.5 %      97.5 %
Mult(Exp(.), orig:dest).educ1         NA          NA
Mult(Exp(.), orig:dest).educ2 -0.5978901  0.1022447
Mult(Exp(.), orig:dest).educ3 -1.4836854 -0.2362378
Mult(Exp(.), orig:dest).educ4 -2.5792398 -0.2953420
Mult(Exp(.), orig:dest).educ5       -Inf -0.7006889
```

5.2 `ofInterest` and `pickCoef`

It is quite common for a statistical model to have a large number of parameters, but for only a subset of these parameters be of interest when it comes to interpreting the model.

The `ofInterest` argument to `gnm` allows the user to specify a subset of the parameters which are of interest, so that *gnm* methods will focus on these parameters. In particular, printed model summaries will only show the parameters of interest, whilst methods for which a subset of parameters may be selected will by default select the parameters of interest, or where this may not be appropriate, provide a *Tk* dialog for selection from the parameters of interest. Parameters may be specified to the `ofInterest` argument by a regular expression to match against parameter names, by a numeric vector of indices, by a character vector of names, or, if `ofInterest = "[?]"` they can be selected through a *Tk* dialog.

The information regarding the parameters of interest is held in the `ofInterest` component of *gnm* objects, which is a named vector of numeric indices, or `NULL` if all parameters are of interest. This component may be accessed or replaced using `ofInterest` or `ofInterest<-` respectively.

The `pickCoef` function provides a simple way to obtain the indices of coefficients from any model object. It takes the model object as its first argument and has an optional `regexp` argument. If a regular expression is passed to `regexp`, the coefficients are selected by matching this regular expression against the coefficient names. Otherwise, coefficients may be selected via a *Tk* dialog.

So, returning to the example from the last section, if we had set `ofInterest` to index the education multipliers as follows

```
ofInterest(unidiff) <- pickCoef(unidiff, "[.]educ")
```

then it would not have been necessary to specify the `which` argument of `profile` as these parameters would have been selected by default.

5.3 `checkEstimable`

The `checkEstimable` function can be used to check the estimability of a linear combination of parameters. For non-linear combinations the same function can be used to check estimability based on the (local) vector of partial derivatives. The `checkEstimable` function provides a numerical version of the sort of algebraic test described in Catchpole and Morgan (1997).

Consider the following model, which is described later in Section 7.3:

```
> doubleUnidiff <- gnm(Freq ~ election:vote + election:class:religion
+                    + Mult(Exp(election), religion:vote) +
+                    Mult(Exp(election), class:vote), family = poisson,
+                    data = cautres)
```

```
Initialising
Running start-up iterations..
Running main iterations..........
Done
```

The effects of the first constituent multiplier in the first multiplicative interaction are identified when the parameter for one of the levels — say for the first level — is constrained to zero. The parameters to be estimated are then the differences between each other level and the first. These differences can be represented by a contrast matrix as follows:

```
> coefs <- names(coef(doubleUnidiff))
> contrCoefs <- coefs[grep(", religion:vote", coefs)]
> nContr <- length(contrCoefs)
> contrMatrix <- matrix(0, length(coefs), nContr,
+                       dimnames = list(coefs, contrCoefs))
> contr <- contr.sum(contrCoefs)
> # switch round to contrast with first level
> contr <- rbind(contr[nContr, ], contr[-nContr, ])
> contrMatrix[contrCoefs, 2:nContr] <- contr
> contrMatrix[contrCoefs, 2:nContr]
```

```
                                        Mult(Exp(.), religion:vote).election2
Mult(Exp(.), religion:vote).election1                                     -1
Mult(Exp(.), religion:vote).election2                                      1
Mult(Exp(.), religion:vote).election3                                      0
Mult(Exp(.), religion:vote).election4                                      0
                                        Mult(Exp(.), religion:vote).election3
Mult(Exp(.), religion:vote).election1                                     -1
Mult(Exp(.), religion:vote).election2                                      0
Mult(Exp(.), religion:vote).election3                                      1
Mult(Exp(.), religion:vote).election4                                      0
                                        Mult(Exp(.), religion:vote).election4
Mult(Exp(.), religion:vote).election1                                     -1
Mult(Exp(.), religion:vote).election2                                      0
Mult(Exp(.), religion:vote).election3                                      0
Mult(Exp(.), religion:vote).election4                                      1
```

Then their estimability can be checked using *checkEstimable*

```
> checkEstimable(doubleUnidiff, contrMatrix)
```

```
Mult(Exp(.), religion:vote).election1 Mult(Exp(.), religion:vote).election2
                                   NA                                  TRUE
Mult(Exp(.), religion:vote).election3 Mult(Exp(.), religion:vote).election4
                                 TRUE                                  TRUE
```

which confirms that the effects for the other three levels are estimable when the parameter for the first level is set to zero.

However, applying the equivalent constraint to the second constituent multiplier in the interaction is not sufficient to make the parameters in that multiplier estimable:

```
> coefs <- names(coef(doubleUnidiff))
> contrCoefs <- coefs[grep("[.]religion", coefs)]
> nContr <- length(contrCoefs)
> contrMatrix <- matrix(0, length(coefs), length(contrCoefs),
+                       dimnames = list(coefs, contrCoefs))
> contr <- contr.sum(contrCoefs)
> contrMatrix[contrCoefs, 2:nContr] <- rbind(contr[nContr, ], contr[-nContr, ])
> checkEstimable(doubleUnidiff, contrMatrix)
```

```
Mult(Exp(election), .).religion1:vote1 Mult(Exp(election), .).religion2:vote1
                                    NA                                 FALSE
Mult(Exp(election), .).religion3:vote1 Mult(Exp(election), .).religion4:vote1
```

```
                                  FALSE                                    FALSE
Mult(Exp(election), .).religion1:vote2 Mult(Exp(election), .).religion2:vote2
                                  FALSE                                    FALSE
Mult(Exp(election), .).religion3:vote2 Mult(Exp(election), .).religion4:vote2
                                  FALSE                                    FALSE
```

5.4 *getContrasts, se*

To investigate simple "sum to zero" contrasts such as those above, it is easiest to use the *getContrasts* function, which checks the estimability of possibly scaled contrasts and returns the parameter estimates with their standard errors. Returning to the example of the first constituent multiplier in the first multiplicative interaction term, the differences between each election and the first can be obtained as follows:

```
> myContrasts <- getContrasts(doubleUnidiff,
+                             pickCoef(doubleUnidiff, ", religion:vote"))
> myContrasts

                                          estimate        SE     quasiSE
Mult(Exp(.), religion:vote).election1   0.0000000 0.0000000 0.09803075
Mult(Exp(.), religion:vote).election2  -0.0878181 0.1136832 0.05702819
Mult(Exp(.), religion:vote).election3  -0.2615200 0.1184134 0.06812239
Mult(Exp(.), religion:vote).election4  -0.3283459 0.1221302 0.07168290
                                            quasiVar
Mult(Exp(.), religion:vote).election1   0.009610029
Mult(Exp(.), religion:vote).election2   0.003252214
Mult(Exp(.), religion:vote).election3   0.004640660
Mult(Exp(.), religion:vote).election4   0.005138439
```

Visualization of estimated contrasts using 'quasi standard errors' (Firth, 2003; Firth and de Menezes, 2004) is achieved by plotting the resulting object:

```
> plot(myContrasts,
+   main = "Relative strength of religion-vote association, log scale",
+ xlab = "Election", levelNames = 1:4)
```

By default, *getContrasts* uses the first parameter of the specified set as the reference level; alternatives may be set via the *ref* argument.

In the above example, the simple contrasts are estimable without scaling. In certain other applications, for example row-column association models (see Section 7.1), the contrasts are identified only after fixing their scale. A more general family of *scaled* contrasts for a set of parameters $\gamma_r, r = 1, \ldots, R$ is given by

$$\gamma_r^* = \frac{\gamma_r - \overline{\gamma}_w}{\sqrt{\sum_r v_r (\gamma_r - \overline{\gamma}_u)^2}}$$

where $\overline{\gamma}_w = \sum w_r \gamma_r$ is the reference level against which the contrasts are taken, $\overline{\gamma}_u = \sum u_r \gamma_r$ is a possibly different weighted mean of the parameters to be used as reference level for a set of "scaling contrasts", and v_r is a further set of weights. Thus, for example, the choice

$$w_r = \begin{cases} 1 & (r = 1) \\ 0 & \text{(otherwise)} \end{cases}, \qquad u_r = v_r = 1/R$$

specifies contrasts with the first level, with the coefficients scaled to have variance 1. This general type of scaling can be obtained by specifying the form of $\overline{\gamma}_u$ and v_r via the *scaleRef* and *scaleWeights* arguments of *getContrasts*.

As an example, consider the following model, described in Section 7.1:

```
> mentalHealth$MHS <- C(mentalHealth$MHS, treatment)
> mentalHealth$SES <- C(mentalHealth$SES, treatment)
> RC1model <- gnm(count ~ SES + MHS + Mult(SES, MHS),
+                 family = poisson, data = mentalHealth)
```

21

Relative strength of religion−vote association, log scale
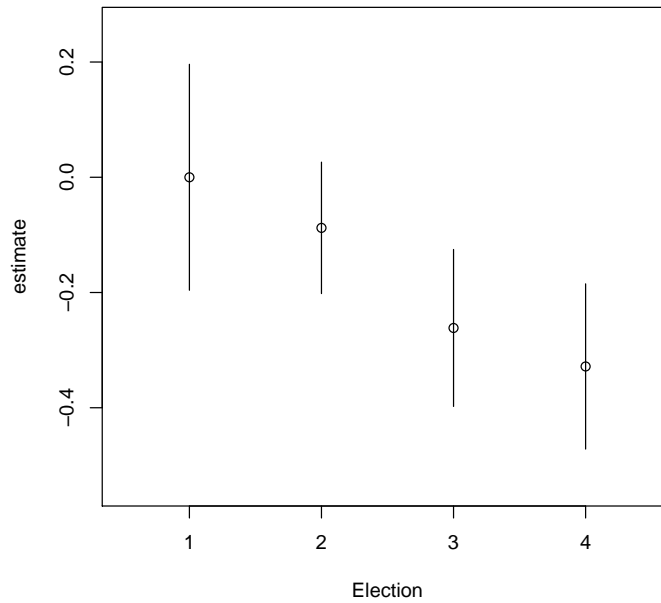
Figure 5: Relative strength of religion-vote association, log scale

```
Initialising
Running start-up iterations..
Running main iterations.......
Done
```

The effects of the constituent multipliers of the multiplicative interaction are identified when both their scale and location are constrained. A simple way to achieve this is to set the first parameter to zero and the last parameter to one:

```
> RC1model2 <- gnm(count ~ SES + MHS + Mult(1, SES, MHS),
+                  constrain = "[.]SES[AF]", constrainTo = c(0, 1),
+                  ofInterest = "[.]SES",
+                  family = poisson, data = mentalHealth)

Initialising
Running start-up iterations..
Running main iterations............
Done

> summary(RC1model2)

Call:

gnm(formula = count ~ SES + MHS + Mult(1, SES, MHS), ofInterest = "[.]SES",
    constrain = "[.]SES[AF]", constrainTo = c(0, 1), family = poisson,
    data = mentalHealth)

Deviance Residuals:
     Min        1Q    Median        3Q       Max
-0.87231  -0.30983   0.01026   0.29898   0.87866
```

```
Coefficients of interest:
                      Estimate Std. Error z value Pr(>|z|)
Mult(1, ., MHS).SESA  0.000000         NA      NA       NA
Mult(1, ., MHS).SESB -0.003107   0.181567  -0.017    0.986
Mult(1, ., MHS).SESC  0.252939   0.158922   1.592    0.111
Mult(1, ., MHS).SESD  0.388785   0.144164   2.697    0.007
Mult(1, ., MHS).SESE  0.724329   0.172325   4.203 2.63e-05
Mult(1, ., MHS).SESF  1.000000         NA      NA       NA


(Dispersion parameter for poisson family taken to be 1)


Std. Error is NA where coefficient has been constrained or is unidentified


Residual deviance: 3.5706 on 8 degrees of freedom
AIC: 179.74


Number of iterations: 12
```

Note that a constant multiplier must be incorporated into the interaction term, i.e., the multiplicative term `Mult(SES, MHS)` becomes `Mult(1, SES, MHS)`, in order to maintain equivalence with the original model specification. The constraints specified for `RC1model2` result in the estimation of scaled contrasts with level *A* of *SES*, in which the scaling fixes the magnitude of the contrast between level *F* and level *A* to be equal to 1. The equivalent use of `getContrasts`, together with the *unconstrained* fit (`RC1model`), in this case is as follows:

```
> getContrasts(RC1model, pickCoef(RC1model, "[.]SES"), ref = "first",
+              scaleRef = "first", scaleWeights = c(rep(0, 5), 1))

                   Estimate Std. Error
Mult(., MHS).SESA  0.000000000  0.0000000
Mult(., MHS).SESB -0.003107289  0.1815672
Mult(., MHS).SESC  0.252939253  0.1589218
Mult(., MHS).SESD  0.388785114  0.1441637
Mult(., MHS).SESE  0.724328752  0.1723247
Mult(., MHS).SESF  1.000000000  0.0000000
```

Quasi-variances and standard errors are not returned here as they can not (currently) be computed for scaled contrasts. When the scaling uses the same reference level as the contrasts, equal scale weights produce "spherical" contrasts, whilst unequal weights produce "elliptical" contrasts. Further examples are given in Sections 7.1 and 7.4.

For more general linear combinations of parameters than contrasts, the lower-level `se` function (which is called internally by `getContrasts` and by the `summary` method) can be used directly. See `help(se)` for details.

5.5 `residSVD`

Sometimes it is useful to operate on the residuals of a model in order to create informative summaries of residual variation, or to obtain good starting values for additional parameters in a more elaborate model. The relevant arithmetical operations are weighted means of the so-called *working residuals*.

The `residSVD` function facilitates one particular residual analysis that is often useful when considering multiplicative interaction between factors as a model elaboration: in effect, `residSVD` provides a direct estimate of the parameters of such an interaction, by performing an appropriately weighted singular value decomposition on the working residuals.

As an illustration, consider the barley data from Wedderburn (1974). These data have the following two-way structure:

```
> xtabs(y ~ site + variety, barley)
```

```
      variety
site      1       2       3       4       5       6       7       8       9       X
   A 0.0005 0.0000 0.0000 0.0010 0.0025 0.0005 0.0050 0.0130 0.0150 0.0150
   B 0.0000 0.0005 0.0005 0.0030 0.0075 0.0030 0.0300 0.0750 0.0100 0.1270
   C 0.0125 0.0125 0.0250 0.1660 0.0250 0.0250 0.0000 0.2000 0.3750 0.2625
   D 0.0250 0.0050 0.0001 0.0300 0.0250 0.0001 0.2500 0.5500 0.0500 0.4000
   E 0.0550 0.0100 0.0600 0.0110 0.0250 0.0800 0.1650 0.2950 0.2000 0.4350
   F 0.0100 0.0500 0.0500 0.0500 0.0500 0.0500 0.1000 0.0500 0.5000 0.7500
   G 0.0500 0.0010 0.0500 0.0500 0.5000 0.1000 0.5000 0.2500 0.5000 0.7500
   H 0.0500 0.1000 0.0500 0.0500 0.2500 0.7500 0.5000 0.7500 0.7500 0.7500
   I 0.1750 0.2500 0.4250 0.5000 0.3750 0.9500 0.6250 0.9500 0.9500 0.9500
```

In Section 7.5 a biplot model is proposed for these data, which comprises a two-component interaction between the cross-classifying factors. In order to fit this model, we can proceed by fitting a smaller model, then use *residSVD* to obtain starting values for the parameters in the bilinear term:

```
> emptyModel <- gnm(y ~ -1, family = wedderburn, data = barley)
> biplotStart <- residSVD(emptyModel, barley$site, barley$variety, d = 2)
> biplotModel <- gnm(y ~ -1 + instances(Mult(site, variety), 2),
+ family = wedderburn, data = barley, start =  biplotStart)

Running main iterations.............................................................
......................................................................
..
Done
```

In this instance, the use of purposive (as opposed to the default, random) starting values had little effect: the fairly large number of iterations needed in this example is caused by a rather flat (quasi-)likelihood surface near the maximum, not by poor starting values. In other situations, the use of *residSVD* may speed the calculations dramatically (see for example Section 7.4), or it may be crucial to success in locating the MLE (for example see *help(House2001)*, where the number of multiplicative parameters is in the hundreds).

The *residSVD* result in this instance provides a crude approximation to the MLE of the enlarged model, as can be seen in Figure 6:

6 *gnm* or *(g)nls*?

The *nls* function in the stats package may be used to fit a nonlinear model via least-squares estimation. Statistically speaking, *gnm* is to *nls* as *glm* is to *lm*, in that a nonlinear least-squares model is equivalent to a generalized nonlinear model with *family = gaussian*. A *nls* model assumes that the responses are distributed either with constant variance or with fixed relative variances (specified via the *weights* argument). The *gnls* function in the nlme package extends *nls* to allow correlated responses. On the other hand, *gnm* allows for responses distributed with variances that are a specified (via the *family* argument) function of the mean; as with *nls*, no correlation is allowed.

The *gnm* function also differs from *nls/gnls* in terms of the interface. Models are specified to *nls* and *gnls* in terms of a mathematical formula or a *selfStart* function based on such a formula, which is convenient for models that have a small number of parameters. For models that have a large number of parameters, or can not easily be represented by a mathematical formula, the symbolic model specification used by *gnm* may be more convenient. This would usually be the case for models involving factors, which would need to be represented by dummy variables in a *nls* formula.

When working with artificial data, *gnm* has the minor advantage that it does not fail when a model is an exact fit to the data (see *help(nls)*). Therefore it is not necessary with *gnm* to add noise to artificial data, which can be useful when testing methods.

Comparison of residSVD and MLE for a 2–dimensional biplot model
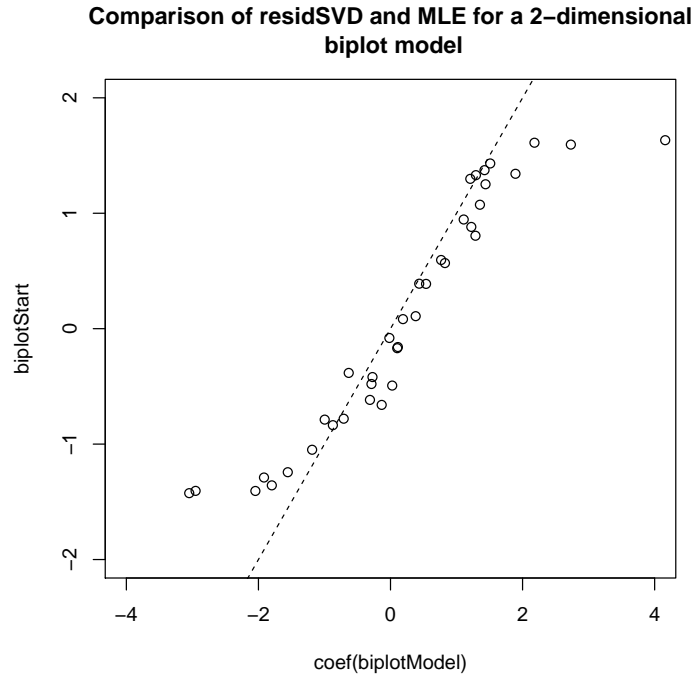
Figure 6: Comparison of residSVD and the MLE for a 2-dimensional biplot model

7 Examples

7.1 Row-column association models

There are several models that have been proposed for modelling the relationship between the cell means of a contingency table and the cross-classifying factors. The following examples consider the row-column association models proposed by Goodman (1979). The examples shown use data from two-way contingency tables, but the gnm package can also be used to fit the equivalent models for higher order tables.

7.1.1 RC(1) model

The RC(1) model is a row and column association model with the interaction between row and column factors represented by one component of the multiplicative interaction. If the rows are indexed by r and the columns by c, then the log-multiplicative form of the RC(1) model for the cell means μ_{rc} is given by

$$\log \mu_{rc} = \alpha_r + \beta_c + \gamma_r \delta_c.$$

We shall fit this model to the `mentalHealth` data set from Agresti (2002, page 381), which is a two-way contingency table classified by the child's mental impairment (MHS) and the parents' socioeconomic status (SES). Although both of these factors are ordered, we do not wish to use polynomial contrasts in the model, so we begin by setting the contrasts attribute of these factors to `treatment`:

```
> set.seed(1)
> mentalHealth$MHS <- C(mentalHealth$MHS, treatment)
> mentalHealth$SES <- C(mentalHealth$SES, treatment)
```

The *gnm* model is then specified as follows, using the poisson family with a log link function:

```
> RC1model <- gnm(count ~ SES + MHS + Mult(SES, MHS), family = poisson,
+                 data = mentalHealth)
```

```
Initialising
Running start-up iterations..
Running main iterations........
Done

> RC1model

Call:
gnm(formula = count ~ SES + MHS + Mult(SES, MHS), family = poisson,
    data = mentalHealth)

Coefficients:
            (Intercept)                  SESB                  SESC
                3.83543              -0.06739               0.10800
                   SESD                  SESE                  SESF
                0.40196               0.01966              -0.20842
                MHSmild            MHSmoderate            MHSimpaired
                0.71188               0.20370               0.24956
      Mult(., MHS).SESA      Mult(., MHS).SESB      Mult(., MHS).SESC
                0.95853               0.96636               0.32099
      Mult(., MHS).SESD      Mult(., MHS).SESE      Mult(., MHS).SESF
               -0.02141              -0.86716              -1.56200
    Mult(SES, .).MHSwell    Mult(SES, .).MHSmild  Mult(SES, .).MHSmoderate
                0.32802               0.03048              -0.02322
 Mult(SES, .).MHSimpaired
               -0.27035


Deviance:              3.570562
Pearson chi-squared:   3.568088
Residual df:           8
```

The row scores (parameters 10 to 15) and the column scores (parameters 16 to 19) of the multiplicative interaction can be normalized as in Agresti's eqn (9.15):

```
> rowProbs <- with(mentalHealth, tapply(count, SES, sum) / sum(count))
> colProbs <- with(mentalHealth, tapply(count, MHS, sum) / sum(count))
> rowScores <- coef(RC1model)[10:15]
> colScores <- coef(RC1model)[16:19]
> rowScores <- rowScores - sum(rowScores * rowProbs)
> colScores <- colScores - sum(colScores * colProbs)
> beta1 <- sqrt(sum(rowScores^2 * rowProbs))
> beta2 <- sqrt(sum(colScores^2 * colProbs))
> assoc <- list(beta = beta1 * beta2,
+               mu = rowScores / beta1,
+               nu = colScores / beta2)
> assoc

$beta
[1] 0.1664874

$mu
Mult(., MHS).SESA Mult(., MHS).SESB Mult(., MHS).SESC Mult(., MHS).SESD
      1.11233085        1.12143706        0.37107608       -0.02702931
Mult(., MHS).SESE Mult(., MHS).SESF
     -1.01036141       -1.81823304


$nu
```

```
    Mult(SES, .).MHSwell        Mult(SES, .).MHSmild Mult(SES, .).MHSmoderate
              1.6775144                   0.1403989               -0.1369926
Mult(SES, .).MHSimpaired
             -1.4136909
```

Alternatively, the elliptical contrasts `mu` and `nu` can be obtained using `getContrasts`, with the advantage that the standard errors for the contrasts will also be computed:

```
> mu <- getContrasts(RC1model, pickCoef(RC1model, "[.]SES"),
+                    ref = rowProbs, scaleWeights = rowProbs)
> nu <- getContrasts(RC1model, pickCoef(RC1model, "[.]MHS"),
+                    ref = colProbs, scaleWeights = colProbs)
> mu

                       Estimate Std. Error
Mult(., MHS).SESA   1.11136052  0.2992108
Mult(., MHS).SESB   1.12045878  0.3142156
Mult(., MHS).SESC   0.37075238  0.3191514
Mult(., MHS).SESD  -0.02700573  0.2732755
Mult(., MHS).SESE  -1.00948003  0.3146991
Mult(., MHS).SESF  -1.81664693  0.2809530

> nu

                        Estimate Std. Error
Mult(SES, .).MHSwell     1.6737834  0.1904282
Mult(SES, .).MHSmild     0.1400866  0.2001792
Mult(SES, .).MHSmoderate -0.1366879  0.2794787
Mult(SES, .).MHSimpaired -1.4105466  0.1741818
```

Since the value of `beta` is dependent upon the particular scaling used for the contrasts, it is typically not of interest to conduct inference on this parameter directly. The standard error for `beta` could be obtained, if desired, via the delta method.

7.1.2 RC(2) model

The RC(1) model can be extended to an RC(m) model with m components of the multiplicative interaction. For example, the RC(2) model is given by

$$\log \mu_{rc} = \alpha_r + \beta_c + \gamma_r \delta_c + \theta_r \phi_c.$$

Extra instances of the multiplicative interaction can be specified by the `multiplicity` argument of `Mult`, so the RC(2) model can be fitted to the `mentalHealth` data as follows

```
> RC2model <- gnm(count ~ SES + MHS + instances(Mult(SES, MHS), 2),
+                 family = poisson, data = mentalHealth)

Initialising
Running start-up iterations..
Running main iterations................
Done

> RC2model

Call:
gnm(formula = count ~ SES + MHS + instances(Mult(SES, MHS), 2),
    family = poisson, data = mentalHealth)

Coefficients:
```

```
                   (Intercept)                                        SESB
                     3.8603353                                   -0.0556106
                          SESC                                        SESD
                     0.1097869                                    0.3284008
                          SESE                                        SESF
                    -0.0381411                                   -0.1524531
                       MHSmild                                 MHSmoderate
                     0.7102765                                    0.1892520
                   MHSimpaired             Mult(., MHS, inst = 1).SESA
                     0.2488493                                   -0.0175314
    Mult(., MHS, inst = 1).SESB      Mult(., MHS, inst = 1).SESC
                    -0.2146166                                   -0.2679378
    Mult(., MHS, inst = 1).SESD      Mult(., MHS, inst = 1).SESE
                     0.8399440                                    0.3076632
    Mult(., MHS, inst = 1).SESF      Mult(SES, ., inst = 1).MHSwell
                    -1.9282818                                    0.6285745
  Mult(SES, ., inst = 1).MHSmild  Mult(SES, ., inst = 1).MHSmoderate
                     0.0791084                                   -0.0465426
Mult(SES, ., inst = 1).MHSimpaired      Mult(., MHS, inst = 2).SESA
                    -0.4539996                                   -0.3575749
    Mult(., MHS, inst = 2).SESB      Mult(., MHS, inst = 2).SESC
                    -0.4908029                                   -0.2886945
    Mult(., MHS, inst = 2).SESD      Mult(., MHS, inst = 2).SESE
                     0.5515182                                    0.5001104
    Mult(., MHS, inst = 2).SESF      Mult(SES, ., inst = 2).MHSwell
                    -0.6576153                                   -0.8149901
  Mult(SES, ., inst = 2).MHSmild  Mult(SES, ., inst = 2).MHSmoderate
                    -0.0092990                                    0.0006713
Mult(SES, ., inst = 2).MHSimpaired
                     0.8711873


Deviance:              0.5225353
Pearson chi-squared: 0.523331
Residual df:           3
```

7.1.3 Homogeneous effects

If the row and column factors have the same levels, or perhaps some levels in common, then the row-column interaction could be modelled by a multiplicative interaction with homogeneous effects, that is

$$\log \mu_{rc} = \alpha_r + \beta_c + \gamma_r \gamma_c.$$

For example, the `occupationalStatus` data set from Goodman (1979) is a contingency table classified by the occupational status of fathers (origin) and their sons (destination). Goodman (1979) fits a row-column association model with homogeneous effects to these data after deleting the cells on the main diagonal. Equivalently we can account for the diagonal effects by a separate `Diag` term:

```
> RChomog <- gnm(Freq ~ origin + destination + Diag(origin, destination) +
+              MultHomog(origin, destination), family = poisson,
+              data = occupationalStatus)

Initialising
Running start-up iterations..
Running main iterations........
Done

> RChomog
```

```
Call:
gnm(formula = Freq ~ origin + destination + Diag(origin, destination) +
    MultHomog(origin, destination), family = poisson, data = occupationalStatus)


Coefficients:
                  (Intercept)                          origin2
                      0.22086                          0.51159
                      origin3                          origin4
                      1.59819                          1.89849
                      origin5                          origin6
                      0.67860                          2.72414
                      origin7                          origin8
                      1.38428                          1.11467
                 destination2                     destination3
                      0.93060                          1.94260
                 destination4                     destination5
                      2.18692                          1.57802
                 destination6                     destination7
                      3.02762                          2.13587
                 destination8          Diag(origin, destination)1
                      1.69005                          1.52667
   Diag(origin, destination)2          Diag(origin, destination)3
                      0.45600                         -0.01598
   Diag(origin, destination)4          Diag(origin, destination)5
                      0.38918                          0.73852
   Diag(origin, destination)6          Diag(origin, destination)7
                      0.13474                          0.45764
   Diag(origin, destination)8     MultHomog(origin, destination)1
                      0.38847                         -1.47122
 MultHomog(origin, destination)2   MultHomog(origin, destination)3
                     -1.25293                         -0.65476
 MultHomog(origin, destination)4   MultHomog(origin, destination)5
                     -0.07088                         -0.05371
 MultHomog(origin, destination)6   MultHomog(origin, destination)7
                      0.45804                          0.87418
 MultHomog(origin, destination)8
                      1.11776

Deviance:             32.56098
Pearson chi-squared:  31.20716
Residual df:          34
```

To determine whether it would be better to allow for heterogeneous effects on the association of the fathers'
occupational status and the sons' occupational status, we can compare this model to the RC(1) model for these
data:

```
> RCheterog <- gnm(Freq ~ origin + destination + Diag(origin, destination) +
+              Mult(origin, destination), family = poisson,
+              data = occupationalStatus)

Initialising
Running start-up iterations..
Running main iterations........
Done

> anova(RChomog, RCheterog)
```

```
Analysis of Deviance Table

Model 1: Freq ~ origin + destination + Diag(origin, destination) + MultHomog(origin,
    destination)
Model 2: Freq ~ origin + destination + Diag(origin, destination) + Mult(origin,
    destination)
  Resid. Df Resid. Dev Df Deviance
1        34     32.561
2        28     29.149  6   3.4118
```

In this case there is little gain in allowing heterogeneous effects.

7.2 Diagonal reference models

Diagonal reference models, proposed by Sobel (1981, 1985), are designed for contingency tables classified by factors with the same levels. The cell means are modelled as a function of the diagonal effects, i.e., the mean responses of the 'diagonal' cells in which the levels of the row and column factors are the same.

Dref example 1: Political consequences of social mobility

To illustrate the use of diagonal reference models we shall use the *voting* data from Clifford and Heath (1993). The data come from the 1987 British general election and are the percentage voting Labour in groups cross-classified by the class of the head of household (*destination*) and the class of their father (*origin*). In order to weight these percentages by the group size, we first back-transform them to the counts of those voting Labour and those not voting Labour:

```
> set.seed(1)
> count <- with(voting, percentage/100 * total)
> yvar <- cbind(count, voting$total - count)
```

The grouped percentages may be modelled by a basic diagonal reference model, that is, a weighted sum of the diagonal effects for the corresponding origin and destination classes. This model may be expressed as

$$\mu_{od} = \frac{e^{\delta_1}}{e^{\delta_1} + e^{\delta_2}}\gamma_o + \frac{e^{\delta_2}}{e^{\delta_1} + e^{\delta_2}}\gamma_d.$$

See Section 3.3 for more detail on the parameterization.

The basic diagonal reference model may be fitted using *gnm* as follows

```
> classMobility <- gnm(yvar ~ Dref(origin, destination),
+                      family = binomial, data = voting)

Initialising
Running main iterations........
Done

> classMobility

Call:
gnm(formula = yvar ~ Dref(origin, destination), family = binomial,
    data = voting)

Coefficients:
                  (Intercept)  Dref(origin, destination)delta1
                     -1.34325                          -0.30736
Dref(origin, destination)delta2   Dref(., .).origin|destination1
                     -0.05501                          -0.83454
 Dref(., .).origin|destination2   Dref(., .).origin|destination3
                      0.21066                          -0.61159
```

```
   Dref(., .).origin|destination4   Dref(., .).origin|destination5
                       0.76500                             1.38370


Deviance:           21.22093
Pearson chi-squared: 18.95311
Residual df:        19
```

and the origin and destination weights can be evaluated as below

```
> DrefWeights(classMobility)

$origin
    weight         se
0.43724694 0.03996404

$destination
    weight         se
0.56275306 0.03996404
```

These results are slightly different from those reported by Clifford and Heath (1993). The reason for this is unclear: we are confident that the above results are correct for the data as given in Clifford and Heath (1993), but have not been able to confirm that the data as printed in the journal were exactly as used in Clifford and Heath's analysis.

Clifford and Heath (1993) suggest that movements in and out of the salariat (class 1) should be treated differently from movements between the lower classes (classes 2 - 5), since the former has a greater effect on social status. Thus they propose the following model

$$
\mu_{od} = \begin{cases}
\dfrac{e^{\delta_1}}{e^{\delta_1} + e^{\delta_2}}\gamma_o + \dfrac{e^{\delta_2}}{e^{\delta_1} + e^{\delta_2}}\gamma_d & \text{if } o = 1 \\[2em]
\dfrac{e^{\delta_3}}{e^{\delta_3} + e^{\delta_4}}\gamma_o + \dfrac{e^{\delta_4}}{e^{\delta_3} + e^{\delta_4}}\gamma_d & \text{if } d = 1 \\[2em]
\dfrac{e^{\delta_5}}{e^{\delta_5} + e^{\delta_6}}\gamma_o + \dfrac{e^{\delta_6}}{e^{\delta_5} + e^{\delta_6}}\gamma_d & \text{if } o \neq 1 \text{ and } d \neq 1
\end{cases}
$$

To fit this model we define factors indicating movement in (upward) and out (downward) of the salariat

```
> upward <- with(voting, origin != 1 & destination == 1)
> downward <- with(voting, origin == 1 & destination != 1)
```

Then the diagonal reference model with separate weights for socially mobile groups can be estimated as follows

```
> socialMobility <- gnm(yvar ~ Dref(origin, destination,
+                                   delta = ~ 1 + downward + upward),
+                        family = binomial, data = voting)

Initialising
Running main iterations........
Done

> socialMobility

Call:
gnm(formula = yvar ~ Dref(origin, destination, delta = ~1 + downward +
    upward), family = binomial, data = voting)

Coefficients:
                                                      (Intercept)
```

```
                                                                  -1.3393
Dref(origin, destination, delta = ~ . + downward + upward).delta1(Intercept)
                                                                   0.1875
        Dref(origin, destination, delta = ~ 1 + . + upward).delta1downwardTRUE
                                                                   0.3442
        Dref(origin, destination, delta = ~ 1 + downward + .).delta1upwardTRUE
                                                                   0.2174
Dref(origin, destination, delta = ~ . + downward + upward).delta2(Intercept)
                                                                   0.5743
        Dref(origin, destination, delta = ~ 1 + . + upward).delta2downwardTRUE
                                                                  -0.4665
        Dref(origin, destination, delta = ~ 1 + downward + .).delta2upwardTRUE
                                                                   0.2776
              Dref(., ., delta = ~ 1 + downward + upward).origin|destination1
                                                                  -0.7183
              Dref(., ., delta = ~ 1 + downward + upward).origin|destination2
                                                                   0.2266
              Dref(., ., delta = ~ 1 + downward + upward).origin|destination3
                                                                  -0.6555
              Dref(., ., delta = ~ 1 + downward + upward).origin|destination4
                                                                   0.7702
              Dref(., ., delta = ~ 1 + downward + upward).origin|destination5
                                                                   1.3969

Deviance:             18.97407
Pearson chi-squared:  17.07493
Residual df:          17
```

The weights for those moving into the salariat, those moving out of the salariat and those in any other group, can be evaluated as below

```
> DrefWeights(socialMobility)

$origin
  downward upward    weight         se
1    FALSE  FALSE 0.4044959 0.05918141
2     TRUE  FALSE 0.6044393 0.12371032
3    FALSE   TRUE 0.3900792 0.08134359


$destination
  downward upward    weight         se
1    FALSE  FALSE 0.5955041 0.05918141
2     TRUE  FALSE 0.3955607 0.12371032
3    FALSE   TRUE 0.6099208 0.08134359
```

Again, the results differ slightly from those reported by Clifford and Heath (1993), but the essence of the results is the same: the origin weight is much larger for the downwardly mobile group than for the other groups. The weights for the upwardly mobile group are very similar to the base level weights, so the model may be simplified by only fitting separate weights for the downwardly mobile group:

```
> downwardMobility <- gnm(yvar ~ Dref(origin, destination,
+                                 delta = ~ 1 + downward),
+                   family = binomial, data = voting)

Initialising
Running main iterations........
Done
```

```
> downwardMobility

Call:
gnm(formula = yvar ~ Dref(origin, destination, delta = ~1 + downward),
    family = binomial, data = voting)

Coefficients:
                                                            (Intercept)
                                                               -1.32007
Dref(origin, destination, delta = ~ . + downward).delta1(Intercept)
                                                                0.05458
     Dref(origin, destination, delta = ~ 1 + .).delta1downwardTRUE
                                                                0.16498
Dref(origin, destination, delta = ~ . + downward).delta2(Intercept)
                                                                0.46337
     Dref(origin, destination, delta = ~ 1 + .).delta2downwardTRUE
                                                               -0.64576
           Dref(., ., delta = ~ 1 + downward).origin|destination1
                                                               -0.74980
           Dref(., ., delta = ~ 1 + downward).origin|destination2
                                                                0.21354
           Dref(., ., delta = ~ 1 + downward).origin|destination3
                                                               -0.67158
           Dref(., ., delta = ~ 1 + downward).origin|destination4
                                                                0.74699
           Dref(., ., delta = ~ 1 + downward).origin|destination5
                                                                1.37637

Deviance:              18.99389
Pearson chi-squared:   17.09981
Residual df:           18

> DrefWeights(downwardMobility)

$origin
  downward    weight         se
1    FALSE 0.3992031 0.04750643
2     TRUE 0.5991570 0.11951340

$destination
  downward    weight         se
1    FALSE 0.6007969 0.04750643
2     TRUE 0.4008430 0.11951340
```

Dref example 2: conformity to parental rules

Another application of diagonal reference models is given by van der Slik et al. (2002). The data from this paper are not publicly available[3], but we shall show how the models presented in the paper may be estimated using *gnm*.

The data relate to the value parents place on their children conforming to their rules. There are two response variables: the mother's conformity score (MCFM) and the father's conformity score (FCFF). The data are cross-classified by two factors describing the education level of the mother (MOPLM) and the father (FOPLF), and there are six further covariates (AGEM, MRMM, FRMF, MWORK, MFCM and FFCF).

In their baseline model for the mother's conformity score, van der Slik et al. (2002) include five of the six covariates (leaving out the father's family conflict score, FCFF) and a diagonal reference term with constant

---

[3] We thank Frans van der Slik for his kindness in sending us the data.

weights based on the two education factors. This model may be expressed as

$$\mu_{rci} = \beta_1 x_{1i} + \beta_2 x_{2i} + \beta_3 x_{3i} + \beta_4 x_{4i} + \beta_5 x_{5i} + \frac{e^{\delta_1}}{e^{\delta_1} + e^{\delta_2}} \gamma_r + \frac{e^{\delta_2}}{e^{\delta_1} + e^{\delta_2}} \gamma_c.$$

The baseline model can be fitted as follows:

```
> set.seed(1)
>  A <- gnm(MCFM ~ -1 + AGEM + MRMM + FRMF + MWORK + MFCM +
+          Dref(MOPLM, FOPLF), family = gaussian, data = conformity,
+          verbose = FALSE)
> A

Call:
gnm(formula = MCFM ~ -1 + AGEM + MRMM + FRMF + MWORK + MFCM +
    Dref(MOPLM, FOPLF), family = gaussian, data = conformity,
    verbose = FALSE)

Coefficients:
                  AGEM                     MRMM                     FRMF
               0.06363                 -0.32425                 -0.25324
                 MWORK                     MFCM     Dref(MOPLM, FOPLF)delta1
              -0.06430                 -0.06043                 -0.33731
Dref(MOPLM, FOPLF)delta2    Dref(., .).MOPLM|FOPLF1    Dref(., .).MOPLM|FOPLF2
              -0.02505                  4.95121                  4.86329
 Dref(., .).MOPLM|FOPLF3    Dref(., .).MOPLM|FOPLF4    Dref(., .).MOPLM|FOPLF5
               4.86458                  4.72343                  4.43516
 Dref(., .).MOPLM|FOPLF6    Dref(., .).MOPLM|FOPLF7
               4.18873                  4.43378

Deviance:             425.3389
Pearson chi-squared:  425.3389
Residual df:          576
```

The coefficients of the covariates are not aliased with the parameters of the diagonal reference term and thus the basic identifiability constraints that have been imposed are sufficient for these parameters to be identified. The diagonal effects do not need to be constrained as they represent contrasts with the off-diagonal cells. Therefore the only unidentified parameters in this model are the weight parameters. This is confirmed in the summary of the model:

```
> summary(A)

Call:
gnm(formula = MCFM ~ -1 + AGEM + MRMM + FRMF + MWORK + MFCM +
    Dref(MOPLM, FOPLF), family = gaussian, data = conformity,
    verbose = FALSE)

Deviance Residuals:
     Min        1Q    Median        3Q       Max
-3.63688  -0.50383   0.01714   0.56753   2.25139

Coefficients:
                      Estimate Std. Error t value Pr(>|t|)
AGEM                   0.06363    0.07375   0.863  0.38859
MRMM                  -0.32425    0.07766  -4.175 3.44e-05
FRMF                  -0.25324    0.07681  -3.297  0.00104
MWORK                 -0.06430    0.07431  -0.865  0.38727
MFCM                  -0.06043    0.07123  -0.848  0.39663
```

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```
Dref(MOPLM, FOPLF)delta1 -0.33731          NA       NA        NA
Dref(MOPLM, FOPLF)delta2 -0.02505          NA       NA        NA
Dref(., .).MOPLM|FOPLF1   4.95121     0.16639   29.757   < 2e-16
Dref(., .).MOPLM|FOPLF2   4.86329     0.10436   46.602   < 2e-16
Dref(., .).MOPLM|FOPLF3   4.86458     0.12855   37.842   < 2e-16
Dref(., .).MOPLM|FOPLF4   4.72343     0.13523   34.929   < 2e-16
Dref(., .).MOPLM|FOPLF5   4.43516     0.19314   22.963   < 2e-16
Dref(., .).MOPLM|FOPLF6   4.18873     0.17142   24.435   < 2e-16
Dref(., .).MOPLM|FOPLF7   4.43378     0.16903   26.231   < 2e-16
---
(Dispersion parameter for gaussian family taken to be 0.7384355)

Std. Error is NA where coefficient has been constrained or is unidentified

Residual deviance: 425.34 on 576 degrees of freedom
AIC: 1507.8

Number of iterations: 15
```

The weights have been constrained to sum to one as described in Section 3.3, so the weights themselves may be estimated as follows:

```
> prop.table(exp(coef(A)[6:7]))

   Dref(MOPLM, FOPLF)delta1 Dref(MOPLM, FOPLF)delta2
                 0.4225638                0.5774362
```

However, in order to estimate corresponding standard errors, the parameters of one of the weights must be constrained. If no such constraints were applied when the model was fitted, `DrefWeights` will refit the model constraining the parameters of the first weight to zero:

```
> DrefWeights(A)

Refitting with parameters of first Dref weight constrained to zero
$MOPLM
    weight        se
0.4225636 0.1439829


$FOPLF
    weight        se
0.5774364 0.1439829
```

giving the values reported by van der Slik et al. (2002). All the other coefficients of model A are the same as those reported by van der Slik et al. (2002) except the coefficients of the mother's gender role (MRMM) and the father's gender role (FRMF). van der Slik et al. (2002) reversed the signs of the coefficients of these factors since they were coded in the direction of liberal values, unlike the other covariates. However, simply reversing the signs of these coefficients does not give the same model, since the estimates of the diagonal effects depend on the estimates of these coefficients. For consistent interpretation of the covariate coefficients, it is better to recode the gender role factors as follows:

```
> MRMM2 <- as.numeric(!conformity$MRMM)
> FRMF2 <- as.numeric(!conformity$FRMF)
> A <- gnm(MCFM ~ -1 + AGEM + MRMM2 + FRMF2 + MWORK + MFCM +
+          Dref(MOPLM, FOPLF), family = gaussian, data = conformity,
+          verbose = FALSE)
> A

Call:
gnm(formula = MCFM ~ -1 + AGEM + MRMM2 + FRMF2 + MWORK + MFCM +
```

```
        Dref(MOPLM, FOPLF), family = gaussian, data = conformity,
        verbose = FALSE)

Coefficients:
                 AGEM                       MRMM2                       FRMF2
              0.06363                     0.32425                     0.25324
                MWORK                        MFCM       Dref(MOPLM, FOPLF)delta1
             -0.06430                    -0.06043                     0.08440
Dref(MOPLM, FOPLF)delta2    Dref(., .).MOPLM|FOPLF1    Dref(., .).MOPLM|FOPLF2
              0.39666                     4.37371                     4.28579
 Dref(., .).MOPLM|FOPLF3    Dref(., .).MOPLM|FOPLF4    Dref(., .).MOPLM|FOPLF5
              4.28708                     4.14593                     3.85767
 Dref(., .).MOPLM|FOPLF6    Dref(., .).MOPLM|FOPLF7
              3.61123                     3.85629

Deviance:            425.3389
Pearson chi-squared: 425.3389
Residual df:              576
```

The coefficients of the covariates are now as reported by van der Slik et al. (2002), but the diagonal effects have been adjusted appropriately.

van der Slik et al. (2002) compare the baseline model for the mother's conformity score to several other models in which the weights in the diagonal reference term are dependent on one of the covariates. One particular model they consider incorporates an interaction of the weights with the mother's conflict score as follows:

$$\mu_{rci} = \beta_1 x_{1i} + \beta_2 x_{2i} + \beta_3 x_{3i} + \beta_4 x_{4i} + \beta_5 x_{5i} + \frac{e^{\xi_{01}+\xi_{11}x_{5i}}}{e^{\xi_{01}+\xi_{11}x_{5i}} + e^{\xi_{02}+\xi_{12}x_{5i}}}\gamma_r + \frac{e^{\xi_{02}+\xi_{12}x_{5i}}}{e^{\xi_{01}+\xi_{11}x_{5i}} + e^{\xi_{02}+\xi_{12}x_{5i}}}\gamma_c.$$

This model can be fitted as below, using the original coding for the gender role factors for ease of comparison to the results reported by van der Slik et al. (2002),

```
> F <- gnm(MCFM ~ -1 + AGEM + MRMM + FRMF + MWORK + MFCM +
+           Dref(MOPLM, FOPLF, delta = ~ 1 + MFCM), family = gaussian,
+           data = conformity, verbose = FALSE)
> F

Call:
gnm(formula = MCFM ~ -1 + AGEM + MRMM + FRMF + MWORK + MFCM +
    Dref(MOPLM, FOPLF, delta = ~1 + MFCM), family = gaussian,
    data = conformity, verbose = FALSE)

Coefficients:
                                                AGEM
                                             0.05818
                                                MRMM
                                            -0.32701
                                                FRMF
                                            -0.25772
                                               MWORK
                                            -0.07847
                                                MFCM
                                            -0.01694
Dref(MOPLM, FOPLF, delta = ~ . + MFCM).delta1(Intercept)
                                             1.03515
        Dref(MOPLM, FOPLF, delta = ~ 1 + .).delta1MFCM
                                            -1.77756
Dref(MOPLM, FOPLF, delta = ~ . + MFCM).delta2(Intercept)
                                            -0.03515
```

```
        Dref(MOPLM, FOPLF, delta = ~ 1 + .).delta2MFCM
                                       2.77756
        Dref(., ., delta = ~ 1 + MFCM).MOPLM|FOPLF1
                                       4.82476
        Dref(., ., delta = ~ 1 + MFCM).MOPLM|FOPLF2
                                       4.88066
        Dref(., ., delta = ~ 1 + MFCM).MOPLM|FOPLF3
                                       4.83969
        Dref(., ., delta = ~ 1 + MFCM).MOPLM|FOPLF4
                                       4.74850
        Dref(., ., delta = ~ 1 + MFCM).MOPLM|FOPLF5
                                       4.42020
        Dref(., ., delta = ~ 1 + MFCM).MOPLM|FOPLF6
                                       4.17957
        Dref(., ., delta = ~ 1 + MFCM).MOPLM|FOPLF7
                                       4.40819


Deviance:            420.9022
Pearson chi-squared: 420.9022
Residual df:         575
```

In this case there are two sets of weights, one for when the mother's conflict score is less than average (coded as zero) and one for when the score is greater than average (coded as one). These can be evaluated as follows:

```
> DrefWeights(F)

Refitting with parameters of first Dref weight constrained to zero
$MOPLM
  MFCM     weight         se
1    1 0.02974675 0.2277711
2    0 0.74465224 0.2006916


$FOPLF
  MFCM    weight         se
1    1 0.9702532 0.2277711
2    0 0.2553478 0.2006916
```

giving the same weights as in Table 4 of van der Slik et al. (2002), though we obtain a lower standard error in the case where MFCM is equal to one.

7.3 Uniform difference (UNIDIFF) models

Uniform difference models (Xie, 1992; Erikson and Goldthorpe, 1992) use a simplified three-way interaction to provide an interpretable model of contingency tables classified by three or more variables. For example, the uniform difference model for a three-way contingency table, also known as the UNIDIFF model, is given by

$$\mu_{ijk} = \alpha_{ik} + \beta_{jk} + \exp(\delta_k)\gamma_{ij}.$$

The γ_{ij} represent a pattern of association that varies in strength over the dimension indexed by k, and $\exp(\delta_k)$ represents the relative strength of that association at level k.

This model can be applied to the *yaish* data set (Yaish, 1998, 2004), which is a contingency table cross-classified by father's social class (*orig*), son's social class (*dest*) and son's education level (*educ*). In this case, we can consider the importance of the association between the social class of father and son across the education levels. We omit the sub-table which corresponds to level 7 of *dest*, because its information content is negligible:

```
> set.seed(1)
> unidiff <- gnm(Freq ~ educ*orig + educ*dest + Mult(Exp(educ), orig:dest),
+               ofInterest = "[.]educ", family = poisson,
+               data = yaish, subset = (dest != 7))
```

```
Initialising
Running start-up iterations..
Running main iterations.......................................
Done

> coef(unidiff)

Coefficients of interest:
Mult(Exp(.), orig:dest).educ1 Mult(Exp(.), orig:dest).educ2
                  -0.05643004                   -0.28180184
Mult(Exp(.), orig:dest).educ3 Mult(Exp(.), orig:dest).educ4
                  -0.79985357                   -1.09536846
Mult(Exp(.), orig:dest).educ5
                  -2.30593233
```

The *ofInterest* component has been set to index the multipliers of the association between the social class of father and son. We can contrast each multiplier to that of the lowest education level and obtain the standard errors for these parameters as follows:

```
> getContrasts(unidiff, ofInterest(unidiff))

                                   estimate        SE    quasiSE    quasiVar
Mult(Exp(.), orig:dest).educ1   0.0000000 0.0000000 0.09757438 0.00952076
Mult(Exp(.), orig:dest).educ2  -0.2253718 0.1611874 0.12885847 0.01660450
Mult(Exp(.), orig:dest).educ3  -0.7434235 0.2335083 0.21182122 0.04486823
Mult(Exp(.), orig:dest).educ4  -1.0389384 0.3434256 0.32609376 0.10633714
Mult(Exp(.), orig:dest).educ5  -2.2495023 0.9453761 0.93560617 0.87535890
```

Four-way contingency tables may sometimes be described by a "double UNIDIFF" model

$$\mu_{ijkl} = \alpha_{il} + \beta_{jkl} + \exp(\delta_l)\gamma_{ij} + \exp(\phi_l)\theta_{ik},$$

where the strengths of two, two-way associations with a common variable are estimated across the levels of the fourth variable. The *cautres* data set, from Cautres et al. (1998), can be used to illustrate the application of the double UNIDIFF model. This data set is classified by the variables vote, class, religion and election. Using a double UNIDIFF model, we can see how the association between class and vote, and the association between religion and vote, differ between the most recent election and the other elections:

```
> set.seed(1)
> doubleUnidiff <- gnm(Freq ~ election*vote + election*class*religion +
+                     Mult(Exp(election), religion:vote) +
+                     Mult(Exp(election), class:vote),
+
+             family = poisson, data = cautres)

Initialising
Running start-up iterations..
Running main iterations...........
Done

> getContrasts(doubleUnidiff, rev(pickCoef(doubleUnidiff, ", class:vote")))

                                       estimate        SE    quasiSE     quasiVar
Mult(Exp(.), class:vote).election4   0.0000000 0.0000000 0.10934796 0.011956977
Mult(Exp(.), class:vote).election3   0.6817374 0.1446833 0.09475939 0.008979341
Mult(Exp(.), class:vote).election2   0.4493744 0.1320022 0.07395886 0.005469914
Mult(Exp(.), class:vote).election1   0.3618303 0.2534754 0.22854401 0.052232364

> getContrasts(doubleUnidiff, rev(pickCoef(doubleUnidiff, ", religion:vote")))
```

```
                                       estimate          SE      quasiSE
Mult(Exp(.), religion:vote).election4  0.0000000 0.00000000 0.07168290
Mult(Exp(.), religion:vote).election3 -0.0878181 0.09906916 0.06812239
Mult(Exp(.), religion:vote).election2 -0.2615200 0.09116479 0.05702819
Mult(Exp(.), religion:vote).election1 -0.3283459 0.12213023 0.09803075
                                       quasiVar
Mult(Exp(.), religion:vote).election4 0.005138439
Mult(Exp(.), religion:vote).election3 0.004640660
Mult(Exp(.), religion:vote).election2 0.003252214
Mult(Exp(.), religion:vote).election1 0.009610029
```

7.4 Generalized additive main effects and multiplicative interaction (GAMMI) models

Generalized additive main effects and multiplicative interaction models, or GAMMI models, were motivated by two-way contingency tables and comprise the row and column main effects plus one or more components of the multiplicative interaction. The singular value corresponding to each multiplicative component is often factored out, as a measure of the strength of association between the row and column scores, indicating the importance of the component, or axis.

For cell means μ_{rc} a GAMMI-K model has the form

$$g(\mu_{rc}) = \alpha_r + \beta_c + \sum_{k=1}^{K} \sigma_k \gamma_{kr} \delta_{kc}, \tag{1}$$

in which g is a link function, α_r and β_c are the row and column main effects, γ_{kr} and δ_{kc} are the row and column scores for multiplicative component k and σ_k is the singular value for component k. The number of multiplicative components, K, is less than or equal to the rank of the matrix of residuals from the main effects.

The row-column association models discussed in Section 7.1 are examples of GAMMI models, with a log link and poisson variance. Here we illustrate the use of an AMMI model, which is a GAMMI model with an identity link and a constant variance.

We shall use the *wheat* data set taken from Vargas et al. (2001), which gives wheat yields measured over ten years. First we scale these yields and create a new treatment factor, so that we can reproduce the analysis of Vargas et al. (2001):

```
> set.seed(1)
> yield.scaled <- wheat$yield * sqrt(3/1000)
> treatment <- interaction(wheat$tillage, wheat$summerCrop, wheat$manure,
+                          wheat$N, sep = "")
```

Now we can fit the AMMI-1 model, to the scaled yields using the combined treatment factor and the year factor from the *wheat* dataset. We will proceed by first fitting the main effects model, then using *residSVD* (see Section 5.5) for the parameters of the multiplicative term:

```
> mainEffects <- gnm(yield.scaled ~ year + treatment, family = gaussian,
+                    data = wheat)
> svdStart <- residSVD(mainEffects, year, treatment, 3)
> bilinear1 <- update(mainEffects, . ~ . + Mult(year, treatment),
+                     start = c(coef(mainEffects), svdStart[,1]))

Running main iterations
Done
```

We can compare the AMMI-1 model to the main effects model,

```
> anova(mainEffects, bilinear1, test = "F")

Analysis of Deviance Table

Model 1: yield.scaled ~ year + treatment
```

```
Model 2: yield.scaled ~ year + treatment + Mult(year, treatment)
  Resid. Df Resid. Dev Df Deviance      F    Pr(>F)
1      207      279515
2      176      128383 31   151133 6.6835 < 2.2e-16
```

giving the same results as in Table 1 of Vargas et al. (2001) (up to error caused by rounding).

Thus the significance of the multiplicative interaction can be tested without applying constraints to this term. If the multiplicative interaction is significant, we may wish to apply constraints to obtain estimates of the row and column scores. We illustrate this using the *barleyHeights* data, which records the average height for 15 genotypes of barley over 9 years.

For this small dataset the AMMI-1 model is easily estimated with the default settings:

```
> set.seed(1)
> barleyModel <- gnm(height ~ year + genotype + Mult(year, genotype),
+                     data = barleyHeights)

Initialising
Running start-up iterations..
Running main iterations.......
Done
```

To obtain the parameterization of Equation 1 in which σ_k is the singular value for component k, the row and column scores must be constrained so that the scores sum to zero and the squared scores sum to one. These contrasts can be obtained using *getContrasts*:

```
> gamma <- getContrasts(barleyModel, pickCoef(barleyModel, "[.]y"),
+                      ref = "mean", scaleWeights = "unit")
> delta <- getContrasts(barleyModel, pickCoef(barleyModel, "[.]g"),
+                      ref = "mean", scaleWeights = "unit")
> gamma
                              Estimate Std. Error
Mult(., genotype).year1974  0.22662083 0.05621029
Mult(., genotype).year1975  0.51350519 0.04856519
Mult(., genotype).year1976  0.43898738 0.05124785
Mult(., genotype).year1977 -0.20046457 0.05658391
Mult(., genotype).year1978 -0.53320298 0.04775769
Mult(., genotype).year1979  0.14181352 0.05724921
Mult(., genotype).year1980 -0.33249439 0.05418746
Mult(., genotype).year1981 -0.17553769 0.05689550
Mult(., genotype).year1982 -0.07922728 0.05770322

> delta
                               Estimate Std. Error
Mult(year, .).genotype1    0.079143300 0.05913864
Mult(year, .).genotype10  -0.335345232 0.05564859
Mult(year, .).genotype11  -0.375909514 0.05466190
Mult(year, .).genotype12   0.285239058 0.05669279
Mult(year, .).genotype13  -0.168316668 0.05843057
Mult(year, .).genotype14   0.293052673 0.05654225
Mult(year, .).genotype15   0.460366625 0.05216774
Mult(year, .).genotype2    0.007543294 0.05933628
Mult(year, .).genotype3    0.169718829 0.05841527
Mult(year, .).genotype4   -0.047168473 0.05926732
Mult(year, .).genotype5    0.181497848 0.05828153
Mult(year, .).genotype6    0.129417613 0.05880326
Mult(year, .).genotype7    0.013581894 0.05933222
Mult(year, .).genotype8   -0.422242966 0.05337051
Mult(year, .).genotype9   -0.270578282 0.05696326
```

Confidence intervals based on the assumption of asymptotic normality can be computed as follows:

```
> gamma[[2]][,1] + (gamma[[2]][,2]) %o% c(-1.96, 1.96)

             [,1]         [,2]
 [1,]  0.11644866  0.33679300
 [2,]  0.41831741  0.60869296
 [3,]  0.33854160  0.53943316
 [4,] -0.31136904 -0.08956010
 [5,] -0.62680805 -0.43959792
 [6,]  0.02960507  0.25402198
 [7,] -0.43870182 -0.22628697
 [8,] -0.28705286 -0.06402252
 [9,] -0.19232559  0.03387103
```

```
> delta[[2]][,1] + (delta[[2]][,2]) %o% c(-1.96, 1.96)

             [,1]         [,2]
 [1,] -0.03676844  0.19505504
 [2,] -0.44441647 -0.22627399
 [3,] -0.48304683 -0.26877219
 [4,]  0.17412119  0.39635693
 [5,] -0.28284059 -0.05379275
 [6,]  0.18222986  0.40387548
 [7,]  0.35811786  0.56261539
 [8,] -0.10875581  0.12384240
 [9,]  0.05522490  0.28421275
[10,] -0.16333242  0.06899548
[11,]  0.06726605  0.29572965
[12,]  0.01416323  0.24467200
[13,] -0.10270926  0.12987305
[14,] -0.52684917 -0.31763677
[15,] -0.38222628 -0.15893028
```

which broadly agree with Table 8 of Chadouef and Denis (1991), allowing for the change in sign.

On the basis of such confidence intervals we can investigate simplifications of the model such as combining levels of the factors or fitting an additive model to a subset of the data.

The singular value σ_k may be obtained as follows

```
> svd(termPredictors(barleyModel)[, "Mult(year, genotype)"])$d
```

```
[1] 43.49601
```

This parameter is of little interest in itself, given that the significance of the term as a whole can be tested using ANOVA.

The SVD representation can also be obtained quite easily for AMMI and GAMMI models with interaction rank greater than 1. See *example(wheat)* for an example of this in an AMMI model with rank 2. (The calculation of *standard errors* and *confidence regions* for the SVD representation with rank greater than 1 is not yet implemented, though.)

7.5 Biplot models

Biplots are graphical displays of two-dimensional arrays, which represent the objects that index both dimensions of the array on the same plot. Here we consider the case of a two-way table, where a biplot may be used to represent both the row and column categories simultaneously.

A two-dimensional biplot is constructed from a rank-2 representation of the data. For two-way tables, the generalized bilinear model defines one such representation:

$$g(\mu_{ij}) = \eta_{ij} = \alpha_{1i}\beta_{1j} + \alpha_{2i}\beta_{2j}$$

since we can alternatively write

$$\boldsymbol{\eta} = \begin{pmatrix} \alpha_{11} & \alpha_{21} \\ \vdots & \vdots \\ \alpha_{1n} & \alpha_{2n} \end{pmatrix} \begin{pmatrix} \beta_{11} & \cdots & \beta_{1p} \\ \beta_{21} & \cdots & \beta_{2p} \end{pmatrix}$$
$$= \boldsymbol{AB}^{T}$$

where the columns of A and B are linearly independent by definition.

To demonstrate how the biplot is obtained from this model, we shall use the `barley` data set which gives the percentage of leaf area affected by leaf blotch for ten varieties of barley grown at nine sites (Wedderburn, 1974; Gabriel, 1998). As suggested by Wedderburn (1974) we model these data using a logit link and a variance proportional to the square of that of the binomial, implemented as the `wedderburn` family in gnm (see also Section 2):

```
> set.seed(83)
> biplotModel <- gnm(y ~ -1 + instances(Mult(site, variety), 2),
+                    family = wedderburn, data = barley)

Initialising
Running start-up iterations..
Running main iterations.......................................................
...................................................................
Done
```

The effect of site i can be represented by the point

$$(\alpha_{1i}, \alpha_{2i})$$

in the space spanned by the linearly independent basis vectors

$$a_1 = (\alpha_{11}, \alpha_{12}, \ldots \alpha_{19})^T$$
$$a_2 = (\alpha_{21}, \alpha_{22}, \ldots \alpha_{29})^T$$

and the variety effects can be similarly represented.

Thus we can represent the sites and varieties separately as follows

```
sites <- pickCoef(biplotModel, "[.]site")
coefs <- coef(biplotModel)
A <- matrix(coefs[sites], nc = 2)
B <- matrix(coefs[-sites], nc = 2)
par(mfrow = c(1, 2))
plot(A, pch = levels(barley$site), xlim = c(-5, 5), ylim = c(-5, 5),
    main = "Site Effects", xlab = "Component 1", ylab = "Component 2")
plot(B, pch = levels(barley$variety), xlim = c(-5, 5), ylim = c(-5, 5),
    main = "Variety Effects", xlab = "Component 1", ylab = "Component 2")
```

Of course the parameterization of the bilinear model is not unique and therefore the scale and rotation of the points in these plots will depend on the random seed. By rotation and reciprocal scaling of the matrices A and B, we can obtain basis vectors with desirable properties without changing the fitted model.

In particular, if we rotate the matrices A and B so that their columns are orthogonal, then the corresponding plots will display the euclidean distances between sites and varieties respectively. If we also scale the matrices A and B so that the corresponding plots have the same units, then we can combine the two plots to give a conventional biplot display.

The required rotation and scaling can be performed via singular value decomposition of the fitted predictors:
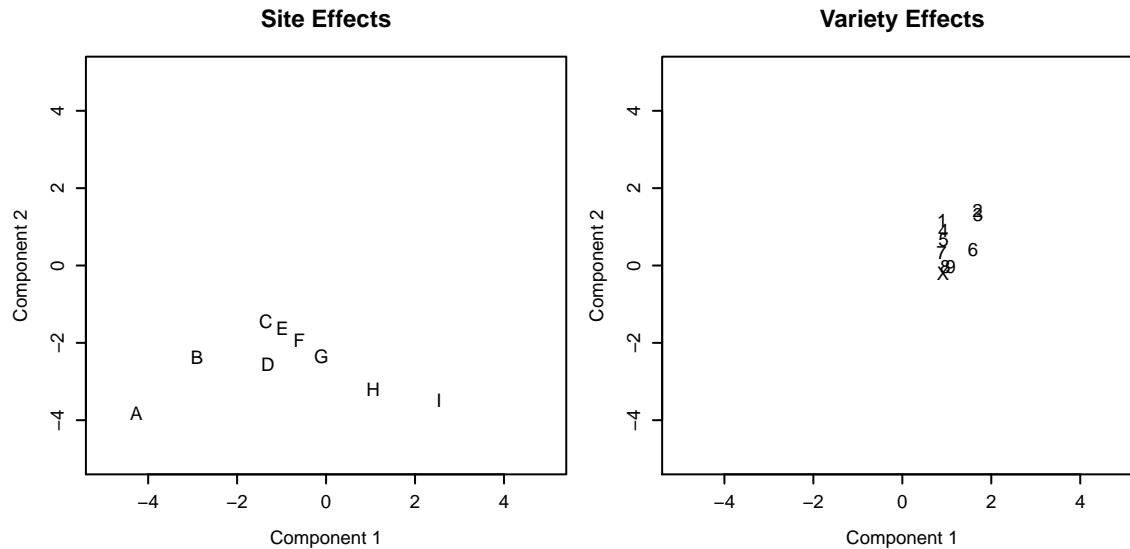
Figure 7: Plots of site and variety effects from the generalized bilinear model of the barley data.

```
> barleyMatrix <- xtabs(biplotModel$predictors ~ site + variety,
+                       data = barley)
> barleySVD <- svd(barleyMatrix)
> A <- sweep(barleySVD$u, 2, sqrt(barleySVD$d), "*")[, 1:2]
> B <- sweep(barleySVD$v, 2, sqrt(barleySVD$d), "*")[, 1:2]
> rownames(A) <- levels(barley$site)
> rownames(B) <- levels(barley$variety)
> colnames(A) <- colnames(B) <- paste("Component", 1:2)
> A

  Component 1 Component 2
A   4.1948225 -0.39186724
B   2.7642412 -0.33951385
C   1.4250454 -0.04654266
D   1.8463067  0.33365989
E   1.2704088  0.15776723
F   1.1562913  0.40048199
G   1.0172048  0.72727987
H   0.6451366  1.46162701
I  -0.1470898  2.13234201

> B

  Component 1 Component 2
1  -2.0673648 -0.97420446
2  -3.0599797 -0.50683007
3  -2.9598031 -0.33190626
4  -1.8086247 -0.49758477
5  -1.5579477 -0.08444511
6  -1.8939995  1.08460553
7  -1.1790432  0.40687014
8  -0.8490092  1.14671349
9  -0.9704664  1.26558202
X  -0.6036789  1.39655881
```

These matrices are essentially the same as in Gabriel (1998). From these the biplot can be produced, for sites $A \ldots I$ and varieties $1 \ldots 9, X$:

```
> barleyCol <- c("red", "blue")
> plot(rbind(A, B), pch = c(levels(barley$site), levels(barley$variety)),
+       col = rep(barleyCol, c(nlevels(barley$site), nlevels(barley$variety))),
+       xlim = c(-4, 4), ylim = c(-4, 4), main = "Biplot for barley data",
+       xlab = "Component 1", ylab = "Component 2")
> text(c(-3.5, -3.5), c(3.9, 3.6), c("sites: A-I","varieties: 1-9, X"),
+       col = barleyCol, adj = 0)
```
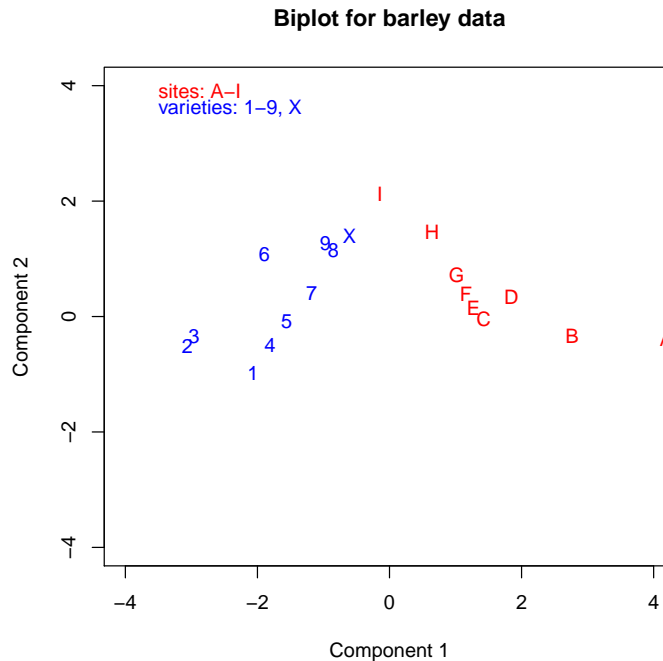

Figure 8: Biplot for barley data

The biplot gives an idea of how the sites and varieties are related to one another. It also allows us to consider whether the data can be represented by a simpler model than the generalized bilinear model. We see that the points in the biplot approximately align with the rotated axes shown in Figure 9, such that the sites fall about a line parallel to the "h-axis" and the varieties group about two lines roughly parallel to the "v-axis".

```
> plot(rbind(A, B), pch = c(levels(barley$site), levels(barley$variety)),
+       col = rep(barleyCol, c(nlevels(barley$site), nlevels(barley$variety))),
+       xlim = c(-4, 4), ylim = c(-4, 4), main = "Biplot for barley data",
+       xlab = "Component 1", ylab = "Component 2")
> text(c(-3.5, -3.5), c(3.9, 3.6), c("sites: A-I","varieties: 1-9, X"),
+       col = barleyCol, adj = 0)
> abline(a = 0, b = tan(pi/3))
> abline(a = 0, b = -tan(pi/6))
> abline(a = 2.6, b = tan(pi/3), lty = 2)
> abline(a = 4.5, b = tan(pi/3), lty = 2)
> abline(a = 1.3, b = -tan(pi/6), lty = 2)
> text(2.8, 3.9, "v-axis", font = 3)
> text(3.8, -2.7, "h-axis", font = 3)
```
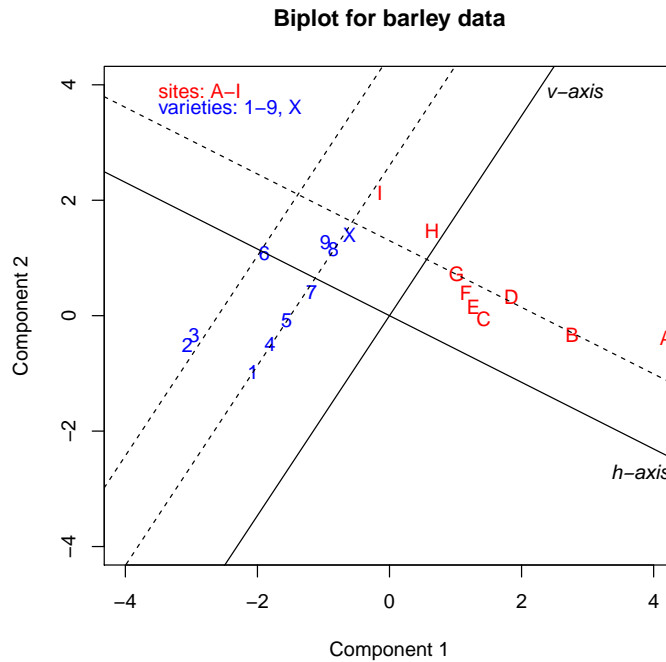
Figure 9: Biplot for barley data, showing approximate alignment with rotated axes.

This suggests that the sites could be represented by points along a line, with co-ordinates

$$(\gamma_i, \delta_0).$$

and the varieties by points on two lines perpendicular to the site line:

$$(\nu_0 + \nu_1 I(i \in \{2, 3, 6\}), \omega_j)$$

This corresponds to the following simplification of the bilinear model:

$$\alpha_{1i}\beta_{1j} + \alpha_{2i}\beta_{2j}$$
$$\approx \gamma_i(\nu_0 + \nu_1 I(i \in \{2, 3, 6\})) + \delta_0\omega_j$$

or equivalently

$$\gamma_i(\nu_0 + \nu_1 I(i \in \{2, 3, 6\})) + \omega_j,$$

the double additive model proposed by Gabriel (1998). We can fit this model as follows:

```
> variety.binary <- factor(match(barley$variety, c(2,3,6), nomatch = 0) > 0,
+                   labels = c("rest", "2,3,6"))
> doubleAdditive <- gnm(y ~ variety + Mult(site, variety.binary),
+                   family = wedderburn, data = barley)

Initialising
Running start-up iterations..
Running main iterations.......................
Done
```

Comparing the chi-squared statistics, we see that the double additive model is an adequate model for the leaf blotch incidence:

```
> biplotModChiSq <- sum(residuals(biplotModel, type = "pearson")^2)
> doubleAddChiSq <- sum(residuals(doubleAdditive, type = "pearson")^2)
> c(doubleAddChiSq - biplotModChiSq,
+    doubleAdditive$df.residual - biplotModel$df.residual)

[1]  9.513773 15.000000
```

7.6 Stereotype model for multinomial response

The stereotype model was proposed by Anderson (1984) for ordered categorical data. It is a special case of the multinomial logistic model, in which the covariate coefficients are common to all categories but the scale of association is allowed to vary between categories such that

$$p_{ic} = \frac{\exp(\beta_{0c} + \gamma_c \boldsymbol{\beta}^T \boldsymbol{x}_i)}{\sum_{k=1}^{K} \exp(\beta_{0k} + \gamma_k \boldsymbol{\beta}^T \boldsymbol{x}_i)}$$

where p_{ic} is the probability that the response for individual i is category c and K is the number of categories. Like the multinomial logistic model, the stereotype model specifies a simple form for the log odds of one category against another, e.g.

$$\log\left(\frac{p_{ic}}{p_{ik}}\right) = (\beta_{0c} - \beta_{0k}) + (\gamma_c - \gamma_k)\boldsymbol{\beta}^T \boldsymbol{x}_i$$

In order to model a multinomial response in the generalized nonlinear model framework, we must re-express the data as category counts $Y_i = (Y_{i1}, \ldots, Y_{iK})$ for each individual (or group). Then assuming a Poisson distribution for the counts Y_{ic}, the joint distribution of Y_i is Multinomial($N_i, p_{i1}, \ldots, p_{iK}$) conditional on the total count for each individual N_i. The expected counts are then $\mu_{ic} = N_i p_{ic}$ and the parameters of the stereotype model can be estimated through fitting the following model

$$\log \mu_{ic} = \log(N_i) + \log(p_{ic})$$
$$= \alpha_i + \beta_{0c} + \gamma_c \sum_r \boldsymbol{\beta}_r \boldsymbol{x}_{ir}$$

where the "nuisance" parameters α_i ensure that the multinomial denominators are reproduced exactly, as required.

The gnm package includes the utility function *expandCategorical* to re-express the categorical response as category counts. By default, individuals with common values across all covariates are grouped together, to avoid redundancy.

For example, the *backPain* data set from Anderson (1984) describes the progress of patients with back pain. The data set consists of an ordered factor quantifying the progress of each patient, and three prognostic variables. We re-express the data as follows:

```
> set.seed(1)
> subset(backPain, x1 == 1 & x2 == 1 & x3 == 1)

   x1 x2 x3                pain
1   1  1  1                same
2   1  1  1 marked.improvement
3   1  1  1    complete.relief
41  1  1  1 marked.improvement
42  1  1  1    complete.relief
43  1  1  1    complete.relief
44  1  1  1    complete.relief

> backPainLong <- expandCategorical(backPain, "pain")
> head(backPainLong)
```

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```
  x1 x2 x3                   pain id count
1  1  1  1                  worse  1     0
2  1  1  1                   same  1     1
3  1  1  1    slight.improvement  1     0
4  1  1  1  moderate.improvement  1     0
5  1  1  1    marked.improvement  1     2
6  1  1  1       complete.relief  1     4
```

We can now fit the stereotype model to these data:

```
> oneDimensional <- gnm(count ~ pain + Mult(pain, x1 + x2 + x3),
+                       eliminate = id, family = "poisson", data = backPainLong)

Initialising
Running start-up iterations..
Running main iterations.............
Done

> oneDimensional

Call:
gnm(formula = count ~ pain + Mult(pain, x1 + x2 + x3), eliminate = id,
    family = "poisson", data = backPainLong)

Coefficients of interest:
                                        painsame
                                         16.1578
                              painslight.improvement
                                         15.6848
                            painmoderate.improvement
                                         12.4556
                              painmarked.improvement
                                         19.9140
                                 paincomplete.relief
                                         21.6653
                 Mult(., x1 + x2 + x3).painworse
                                          0.3322
                  Mult(., x1 + x2 + x3).painsame
                                         -1.9147
   Mult(., x1 + x2 + x3).painslight.improvement
                                         -1.7935
 Mult(., x1 + x2 + x3).painmoderate.improvement
                                         -1.2625
   Mult(., x1 + x2 + x3).painmarked.improvement
                                         -2.4609
     Mult(., x1 + x2 + x3).paincomplete.relief
                                         -2.9214
                      Mult(pain, . + x2 + x3).x1
                                          1.6510
                      Mult(pain, x1 + . + x3).x2
                                          0.9470
                      Mult(pain, x1 + x2 + .).x3
                                          0.8338


Deviance:            55.90786
Pearson chi-squared: 49.61719
Residual df:         48
```

specifying the `id` factor through `eliminate` so that the 12 `id` effects are estimated more efficiently and are excluded from printed model summaries by default. This model is one dimensional since it involves only one function of $\mathbf{x} = (x1, x2, x3)$. We can compare this model to one with category-specific coefficients of the x variables, as may be used for a qualitative categorical response:

```
> threeDimensional  <- gnm(count ~ pain + pain:(x1 + x2 + x3), eliminate = id,
+                          family = "poisson", data = backPainLong)
> threeDimensional

Call:
gnm(formula = count ~ pain + pain:(x1 + x2 + x3), eliminate = id,
    family = "poisson", data = backPainLong)

Coefficients of interest:
                      painsame       painslight.improvement
                       34.3281                      33.9473
    painmoderate.improvement        painmarked.improvement
                       30.8299                      38.0305
         paincomplete.relief                   painworse:x1
                       40.4785                      14.4127
                   painsame:x1    painslight.improvement:x1
                        1.7421                       2.0717
 painmoderate.improvement:x1    painmarked.improvement:x1
                        2.3351                       0.5119
      paincomplete.relief:x1                   painworse:x2
                            NA                       3.2750
                   painsame:x2    painslight.improvement:x2
                        0.6009                       0.7236
 painmoderate.improvement:x2    painmarked.improvement:x2
                        1.6029                       0.4311
      paincomplete.relief:x2                   painworse:x3
                            NA                       2.9406
                   painsame:x3    painslight.improvement:x3
                        1.7852                       1.6486
 painmoderate.improvement:x3    painmarked.improvement:x3
                        2.1944                       1.2491
      paincomplete.relief:x3
                            NA

Deviance:            51.82277
Pearson chi-squared: 43.86631
Residual df:         40
```

This model has the maximum dimensionality of three (as determined by the number of covariates). The ungrouped multinomial log-likelihoods reported in Anderson (1984) are given by

$$\sum_{i,c} y_{ic} \log(p_{ic}) = \sum_{i,c} y_{ic} \log(\mu_{ic}/n_{ic})$$

We write a simple function to compute this and the corresponding degrees of freedom, then compare the log-likelihoods of the one dimensional model and the three dimensional model:

```
> logLikMultinom <- function(model, size){
+     object <- get(model)
+     l <- sum(object$y * log(object$fitted/size))
+     c(nParameters = object$rank - nlevels(object$eliminate), logLikelihood = l)
+ }
> size <- tapply(backPainLong$count, backPainLong$id, sum)[backPainLong$id]
> t(sapply(c("oneDimensional", "threeDimensional"), logLikMultinom, size))
```

```
               nParameters logLikelihood
oneDimensional          12     -151.5501
threeDimensional        20     -149.5076
```

showing that the *oneDimensional* model is adequate.

To obtain estimates of the category-specific multipliers in the stereotype model, we need to constrain both the location and the scale of these parameters. The latter constraint can be imposed by fixing the slope of one of the covariates in the second multiplier to *1*, which may be achieved by specifying the covariate as an offset:

```
> ## before constraint
> summary(oneDimensional)

Call:
gnm(formula = count ~ pain + Mult(pain, x1 + x2 + x3), eliminate = id,
    family = "poisson", data = backPainLong)

Deviance Residuals:
    Min      1Q   Median      3Q     Max
-2.0335  -0.9195  -0.1354  0.3593  1.7115

Coefficients of interest:
                                             Estimate Std. Error z value
painsame                                      16.1578     6.5741   2.458
painslight.improvement                        15.6848     6.5274   2.403
painmoderate.improvement                      12.4556     6.4312   1.937
painmarked.improvement                        19.9140     6.4975   3.065
paincomplete.relief                           21.6653     6.5571   3.304
Mult(., x1 + x2 + x3).painworse                0.3322         NA      NA
Mult(., x1 + x2 + x3).painsame                -1.9147         NA      NA
Mult(., x1 + x2 + x3).painslight.improvement  -1.7935         NA      NA
Mult(., x1 + x2 + x3).painmoderate.improvement -1.2625        NA      NA
Mult(., x1 + x2 + x3).painmarked.improvement  -2.4609         NA      NA
Mult(., x1 + x2 + x3).paincomplete.relief     -2.9214         NA      NA
Mult(pain, . + x2 + x3).x1                      1.6510         NA      NA
Mult(pain, x1 + . + x3).x2                      0.9470         NA      NA
Mult(pain, x1 + x2 + .).x3                      0.8338         NA      NA
                                             Pr(>|z|)
painsame                                      0.013980
painslight.improvement                        0.016265
painmoderate.improvement                      0.052777
painmarked.improvement                        0.002178
paincomplete.relief                           0.000953
Mult(., x1 + x2 + x3).painworse                     NA
Mult(., x1 + x2 + x3).painsame                      NA
Mult(., x1 + x2 + x3).painslight.improvement        NA
Mult(., x1 + x2 + x3).painmoderate.improvement      NA
Mult(., x1 + x2 + x3).painmarked.improvement        NA
Mult(., x1 + x2 + x3).paincomplete.relief           NA
Mult(pain, . + x2 + x3).x1                          NA
Mult(pain, x1 + . + x3).x2                          NA
Mult(pain, x1 + x2 + .).x3                          NA

(Dispersion parameter for poisson family taken to be 1)

Std. Error is NA where coefficient has been constrained or is unidentified

Residual deviance: 55.908 on 48 degrees of freedom
```

```
AIC: 211.81

Number of iterations: 14

> oneDimensional <- gnm(count ~ pain + Mult(pain, offset(x1) + x2 + x3),
+                      eliminate = id, family = "poisson", data = backPainLong)

Initialising
Running start-up iterations..
Running main iterations.............
Done

> ## after constraint
> summary(oneDimensional)

Call:
gnm(formula = count ~ pain + Mult(pain, offset(x1) + x2 + x3),
    eliminate = id, family = "poisson", data = backPainLong)

Deviance Residuals:
    Min      1Q   Median      3Q      Max
-2.0335  -0.9195  -0.1354   0.3593   1.7115

Coefficients of interest:
                                                        Estimate Std. Error
painsame                                                 16.1578     6.5742
painslight.improvement                                   15.6848     6.5274
painmoderate.improvement                                 12.4556     6.4312
painmarked.improvement                                   19.9140     6.4976
paincomplete.relief                                      21.6654     6.5571
Mult(., x2 + x3 + offset(x1)).painworse                   1.4679         NA
Mult(., x2 + x3 + offset(x1)).painsame                   -2.2419         NA
Mult(., x2 + x3 + offset(x1)).painslight.improvement     -2.0418         NA
Mult(., x2 + x3 + offset(x1)).painmoderate.improvement   -1.1651         NA
Mult(., x2 + x3 + offset(x1)).painmarked.improvement     -3.1437         NA
Mult(., x2 + x3 + offset(x1)).paincomplete.relief        -3.9040         NA
Mult(pain, . + x3 + offset(x1)).x2                         0.5736     0.2178
Mult(pain, x2 + . + offset(x1)).x3                         0.5050     0.2431
                                                        z value Pr(>|z|)
painsame                                                  2.458 0.013980
painslight.improvement                                    2.403 0.016265
painmoderate.improvement                                  1.937 0.052777
painmarked.improvement                                    3.065 0.002178
paincomplete.relief                                       3.304 0.000953
Mult(., x2 + x3 + offset(x1)).painworse                      NA       NA
Mult(., x2 + x3 + offset(x1)).painsame                       NA       NA
Mult(., x2 + x3 + offset(x1)).painslight.improvement         NA       NA
Mult(., x2 + x3 + offset(x1)).painmoderate.improvement       NA       NA
Mult(., x2 + x3 + offset(x1)).painmarked.improvement         NA       NA
Mult(., x2 + x3 + offset(x1)).paincomplete.relief           NA       NA
Mult(pain, . + x3 + offset(x1)).x2                         2.633 0.008451
Mult(pain, x2 + . + offset(x1)).x3                         2.077 0.037808

(Dispersion parameter for poisson family taken to be 1)

Std. Error is NA where coefficient has been constrained or is unidentified
```

```
Residual deviance: 55.908 on 48 degrees of freedom
AIC: 211.81

Number of iterations: 14
```

The location of the category-specific multipliers can constrained by setting one of the parameters to zero, either through the *constrain* argument of *gnm* or with *getContrasts*:

```
> getContrasts(oneDimensional, pickCoef(oneDimensional, "[.]pain"))

                                                      estimate       SE
Mult(., x2 + x3 + offset(x1)).painworse              0.000000 0.000000
Mult(., x2 + x3 + offset(x1)).painsame              -3.709738 1.825568
Mult(., x2 + x3 + offset(x1)).painslight.improvement -3.509697 1.791732
Mult(., x2 + x3 + offset(x1)).painmoderate.improvement -2.632943 1.669256
Mult(., x2 + x3 + offset(x1)).painmarked.improvement -4.611597 1.895240
Mult(., x2 + x3 + offset(x1)).paincomplete.relief   -5.371854 1.999657
                                                       quasiSE  quasiVar
Mult(., x2 + x3 + offset(x1)).painworse              1.7797353 3.16745779
Mult(., x2 + x3 + offset(x1)).painsame               0.4281334 0.18329821
Mult(., x2 + x3 + offset(x1)).painslight.improvement 0.4024684 0.16198083
Mult(., x2 + x3 + offset(x1)).painmoderate.improvement 0.5518548 0.30454368
Mult(., x2 + x3 + offset(x1)).painmarked.improvement 0.3133220 0.09817066
Mult(., x2 + x3 + offset(x1)).paincomplete.relief    0.4919550 0.24201969
```

giving the required estimates.

7.7 Lee-Carter model for trends in age-specific mortality

In the study and projection of population mortality rates, the model proposed by Lee and Carter (1992) forms the basis of many if not most current analyses. Here we consider the quasi-Poisson version of the model (Wilmoth, 1993; Alho, 2000; Brouhns et al., 2002; Renshaw and Haberman, 2003), in which the death count D_{ay} for individuals of age a in year y has mean μ_{ay} and variance $\phi\mu_{ay}$ (where ϕ is 1 for Poisson-distributed counts, and is respectively greater than or less than 1 in cases of over-dispersion or under-dispersion). In the Lee-Carter model, the expected counts follow the log-bilinear form

$$\log(\mu_{ay}/e_{ay}) = \alpha_a + \beta_a\gamma_y,$$

where e_{ay} is the 'exposure' (number of lives at risk). This is a generalized nonlinear model with a single multiplicative term.

The use of gnm to fit this model is straightforward. We will illustrate by using data downloaded on 2006-11-14 from the Human Mortality Database[4] (HMD, made available by the University of California, Berkeley, and Max Planck Institute for Demographic Research, at http://www.mortality.org) on male deaths in Canada between 1921 and 2003. The data are not made available as part of gnm because of license restrictions; but they are readily available via the web simply by registering with the HMD. We assume that the data for Canadian males (both deaths and exposure-to-risk) have been downloaded from the HMD and organised into a data frame named *Canada* in R, with columns *Year* (a factor, with levels *1921* to *2003*), *Age* (a factor, with levels *20* to *99*), *mDeaths* and *mExposure* (both quantitative). The Lee-Carter model may then be specified as

```
LCmodel.male <- gnm(mDeaths ~ Age + Mult(Exp(Age), Year),
                offset = log(mExposure), family = "quasipoisson",
                data = Canada)
```

Here we have acknowledged the fact that the model only really makes sense if all of the β_a parameters, which represent the 'sensitivity' of age group a to a change in the level of general mortality (e.g., Brouhns et al., 2002), have the same sign. Without loss of generality we assume $\beta_a > 0$ for all a, and we impose this constraint by using *Exp(Age)* instead of just *Age* in the multiplicative term. Convergence is to a fitted model with residual deviance

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[4]Thanks to Iain Currie for helpful advice relating to this section

32419.83 on 6399 degrees of freedom — representing clear evidence of substantial overdispersion relative to the Poisson distribution. In order to explore the lack of fit a little further, we plot the distribution of Pearson residuals in Figure 10:

```
par(mfrow = c(2,2))
age <- as.numeric(as.character(Canada$Age))
with(Canada,{
    res <- residuals(LCmodel.male, type = "pearson")
    plot(Age, res, xlab="Age", ylab="Pearson residual",
        main = "(a) Residuals by age")
    plot(Year, res, xlab="Year", ylab="Pearson residual",
        main = "(b) Residuals by year")
    plot(Year[(age>24) & (age<36)], res[(age>24) & (age<36)],
        xlab = "Year", ylab = "Pearson residual",
        main = "(c) Age group 25-35")
    plot(Year[(age>49) & (age<66)], res[(age>49) & (age<66)],
        xlab = "Year", ylab = "Pearson residual",
        main = "(d) Age group 50-65")
})
```

Panel (a) of Figure 10 indicates that the overdispersion is not evenly spread through the data, but is largely concentrated in two age groups, roughly ages 25–35 and 50–65. Panels (c) and (d) focus on the residuals in each of these two age groups: there is a clear (and roughly cancelling) dependence on *Year*, indicating that the assumed bilinear interaction between *Age* and *Year* does not hold for the full range of ages and years considered here.

A somewhat more satisfactory Lee-Carter model fit is obtained if only a subset of the data is used, namely only those males aged 45 or over:

```
LCmodel.maleOver45 <- gnm(mDeaths ~ Age + Mult(Exp(Age), Year),
                          offset = log(mExposure), family = "quasipoisson",
                          data = Canada[age>44,])
```

The residual deviance now is 12595.44 on 4375 degrees of freedom: still substantially overdispersed, but less severely so than before. Again we plot the distributions of Pearson residuals (Figure 11). Still clear departures from the assumed bilinear structure are evident, especially for age group 81–89; but they are less pronounced than in the previous model fit.

The main purpose here is only to illustrate how straightforward it is to work with the Lee-Carter model using *gnm*, but we will take this example a little further by examining the estimated β_a parameters from the last fitted model. We can use *getContrasts* to compute quasi standard errors for the logarithms of $\hat{\beta}_a$ — the logarithms being the result of having used *Exp(Age)* in the model specification — and use these in a plot of the coefficients:

```
AgeContrasts <- getContrasts(LCmodel.maleOver45, 56:100) ## ages 45 to 89 only
```

The plot shows that sensitivity to the general level of mortality is highest at younger ages, as expected. An *unexpected* feature is the clear outlying positions occupied by the estimates for ages 51, 61, 71 and 81: for each of those ages, the estimated β_a coefficient is substantially less than it is for the neighbouring age groups (and the error bars indicate clearly that the deviations are larger than could plausibly be due to chance variation). This is a curious finding. An explanation comes from a look back at the raw death-count data. In the years between 1921 and 1940, the death counts for ages 31, 41, 51, 61, 71 and 81 all stand out as being very substantially lower than those of neighbouring ages (Figure 13: the ages concerned are highlighted in solid red). The same does *not* hold for later years: after about 1940, the '1' ages fall in with the general pattern. This apparent 'age heaping[5]' explains our finding above regarding the β_a coefficients: whilst all age groups have benefited from the general trend of reduced mortality, the '1' age groups appear to have benefited least because their starting point (in the 1920s and 1930s) was lower than would have been indicated by the general pattern — hence $\hat{\beta}_a$ is smaller for ages $a = 31$, $a = 41$,..., $a = 81$.

---

[5]Age heaping is common in mortality data: see http://www.mortality.org/Public/Overview.php
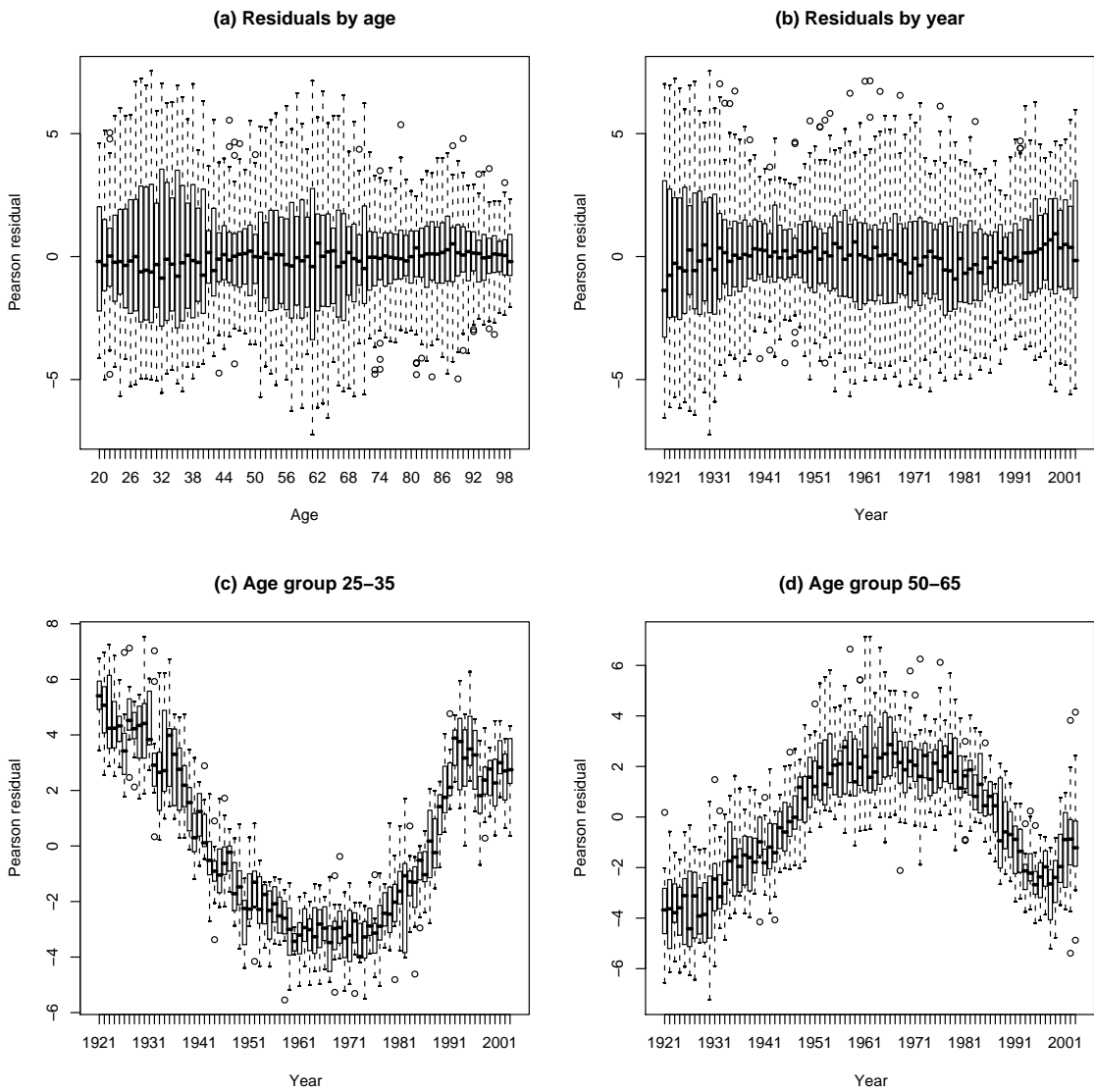
52

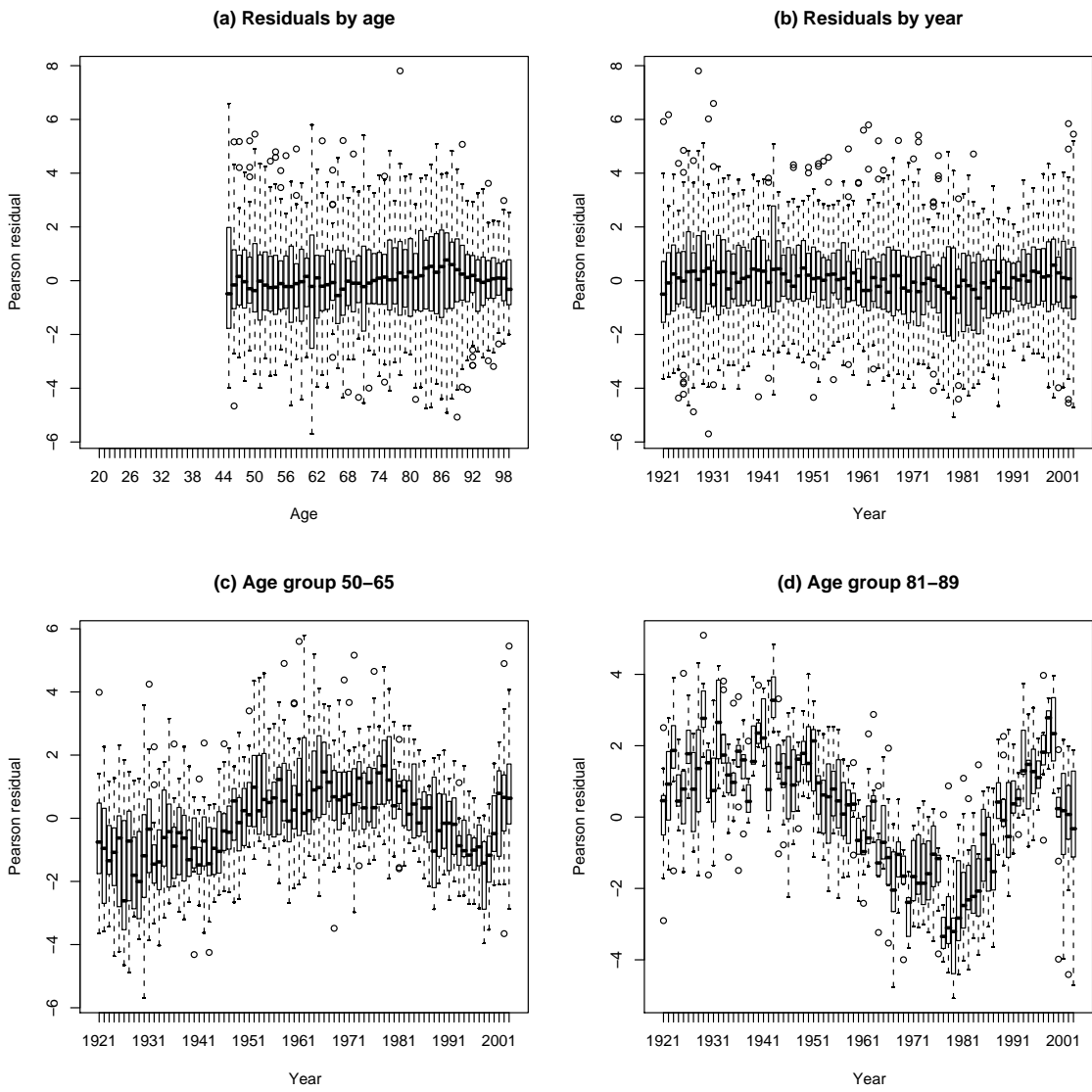Figure 10: Canada, males: plots of residuals from the Lee-Carter model of mortality

Figure 11: Canada, males over 45: plots of residuals from the Lee-Carter model of mortality
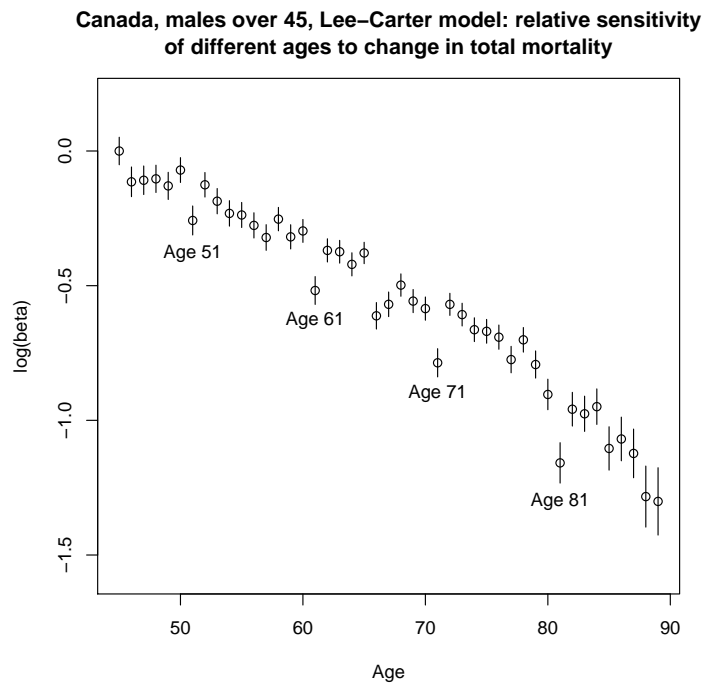
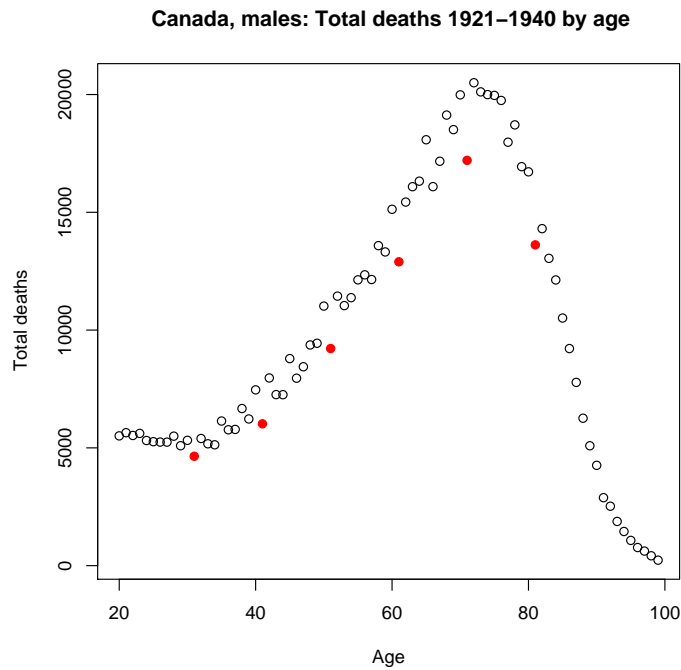**Canada, males over 45, Lee–Carter model: relative sensitivity of different ages to change in total mortality**

Figure 12: Canada, males over 45, Lee-Carter model: relative sensitivity of different ages to change in total mortality.

Canada, males: Total deaths 1921–1940 by age

Figure 13: Canada, males: Deaths 1921 to 1940 by age

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7.8 Exponential and sum-of-exponentials models for decay curves

A class of nonlinear functions which arise in various application contexts — a notable one being pharmacokinetic studies – involves one or more *exponential decay* terms. For example, a simple decay model with additive error is

$$y = \alpha + \exp(\beta + \gamma x) + e \tag{2}$$

(with $\gamma < 0$), while a more complex ('sum of exponentials') model might involve two decay terms:

$$y = \alpha + \exp(\beta_1 + \gamma_1 x) + \exp(\beta_2 + \gamma_2 x) + e. \tag{3}$$

Estimation and inference with such models are typically not straightforward, partly on account of multiple local maxima in the likelihood (e.g., Seber and Wild, 1989, Ch.3). We illustrate the difficulties here, with a couple of artificial examples. These examples will make clear the value of making repeated calls to *gnm*, in order to use different, randomly-generated parameterizations and starting values and thus improve the chances of locating both the global maximum and all local maxima of the likelihood.

7.8.1 Example: single exponential decay term

Let us first construct some data from model (2). For our illustrative purposes here, we will use *noise-free* data, i.e., we fix the variance of e to be zero; for the other parameters we will use $\alpha = 0, \beta = 0, \gamma = -0.1$.

```
> x <- 1:100
> y <- exp(- x / 10)
> set.seed(1)
> saved.fits <- list()
> for (i in 1:100) saved.fits[[i]] <- gnm(y ~ Exp(1 + x), verbose = FALSE)
> table(zapsmall(sapply(saved.fits, deviance)))

      0 3.612654
     52       48
```

The `saved.fits` object thus contains the results of 100 calls to *gnm*, each using a different, randomly-generated starting value for the vector of parameters (α, β, γ). Out of 100 fits, 52 reproduce the data exactly, to machine accuracy. The remaining 48 fits are all identical to one another, but they are far from globally optimal, with residual sum of squares 3.61: they result from divergence of $\hat{\gamma}$ to $+\infty$, and correspondingly of $\hat{\beta}$ to $-\infty$, such that the fitted 'curve' is in fact just a constant, with level equal to $\bar{y} = 0.09508$. For example, the second of the 100 fits is of this kind:

```
> saved.fits[[2]]

Call:
gnm(formula = y ~ Exp(1 + x), verbose = FALSE)

Coefficients:
          (Intercept)  Exp(. + x).(Intercept)             Exp(1 + .).x
            9.508e-02                -1.493e+04                5.463e+01

Deviance:            3.612654
Pearson chi-squared: 3.612654
Residual df:         99
```

The use of repeated calls to *gnm*, as here, allows the local and global maxima to be easily distinguished.

7.8.2 Example: sum of two exponentials

We can conduct a similar exercise based on the more complex model (3):

```
> x <- 1:100
> y <- exp(- x / 10) + 2 * exp(- x / 50)
> set.seed(1)
> saved.fits <- list()
> for (i in 1:100) {
+     saved.fits[[i]] <- suppressWarnings(gnm(y ~ Exp(1 + x, inst = 1) +
+                                             Exp(1 + x, inst = 2),
+                                             verbose = FALSE))
+ }
> table(round(unlist(sapply(saved.fits, deviance)), 4))

     0  0.1589 41.6439
    20       3       4
```

In this instance, only 27 of the 100 calls to *gnm* have successfully located a local maximum of the likelihood: in the remaining 73 cases the starting values generated were such that numerical problems resulted, and the fitting algorithm was abandoned (giving a *NULL* result). Among the 27 'successful' fits, it is evident that there are three distinct solutions (with respective residual sums of squares equal to 0.1589, 41.64, and essentially zero — the last of these, the exact fit to the data, having been found 20 times out of the above 27). The two non-optimal local maxima here correspond to the best fit with a single exponential (which has residual sum of squares 0.1589) and to the fit with no dependence at all on *x* (residual sum of squares 41.64), as we can see by comparing with:

```
> singleExp <- gnm(y ~ Exp(1 + x), start = c(NA, NA, -0.1), verbose = FALSE)
> singleExp

Call:
gnm(formula = y ~ Exp(1 + x), start = c(NA, NA, -0.1), verbose = FALSE)

Coefficients:
          (Intercept)  Exp(. + x).(Intercept)          Exp(1 + .).x
              0.25007                 0.93664              -0.03465

Deviance:            0.1589496
Pearson chi-squared: 0.1589496
Residual df:         97

> meanOnly <- gnm(y ~ 1, verbose = FALSE)
> meanOnly

Call:
gnm(formula = y ~ 1, verbose = FALSE)

Coefficients:
(Intercept)
     0.9511

Deviance:            41.6439
Pearson chi-squared: 41.6439
Residual df:         99

> plot(x, y, main = "Two sub-optimal fits to a sum-of-exponentials curve")
> lines(x, fitted(singleExp))
> lines(x, fitted(meanOnly), lty = "dashed")
```

In this example, it is clear that even a small amount of noise in the data would make it practically impossible to distinguish between competing models containing one and two exponential-decay terms.

In summary: the default *gnm* setting of randomly-chosen starting values is useful for identifying multiple local maxima in the likelihood; and reasonably good starting values are needed if the global maximum is to be found. In the present example, knowing that γ_1 and γ_2 should both be small and negative, we might perhaps have tried

Two sub–optimal fits to a sum–of–exponentials curve
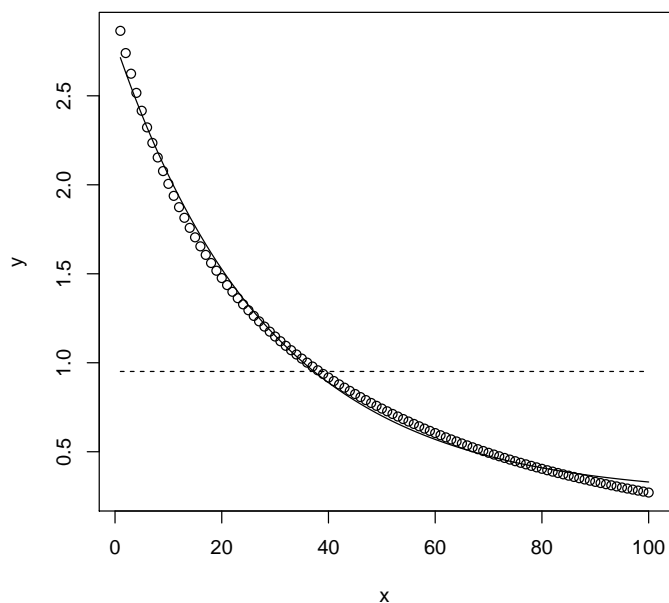

Figure 14: Two sub-optimal fits to a sum-of-exponentials curve

```
> gnm(y ~ instances(Exp(1 + x), 2), start = c(NA, NA, -0.1, NA, -0.1),
+       verbose = FALSE)

Call:
gnm(formula = y ~ instances(Exp(1 + x), 2), start = c(NA, NA,
    -0.1, NA, -0.1), verbose = FALSE)

Coefficients:
                      (Intercept)  Exp(. + x, inst = 1).(Intercept)
                        2.059e-12                        -3.924e-12
         Exp(1 + ., inst = 1).x  Exp(. + x, inst = 2).(Intercept)
                       -1.000e-01                         6.931e-01
         Exp(1 + ., inst = 2).x
                       -2.000e-02

Deviance:            2.922785e-24
Pearson chi-squared: 2.922785e-24
Residual df:         95
```

which reliably yields the (globally optimal) perfect fit to the data.

A User-level functions

We list here, for easy reference, all of the user-level functions in the gnm package. For full documentation see the package help pages.

Model Fitting	
gnm	fit generalized nonlinear models

Model Specification	
Diag	create factor differentiating diagonal elements
Symm	create symmetric interaction of factors
Topo	create 'topological' interaction factors
Const	specify a constant in a *nonlin* function predictor
Dref	specify a diagonal reference term in a **gnm** model formula
Mult	specify a product of predictors in a **gnm** formula
MultHomog	specify a multiplicative interaction with homogeneous effects in a **gnm** formula
Exp	specify the exponential of a predictor in a **gnm** formula
Inv	specify the reciprocal of a predictor in a **gnm** formula
wedderburn	specify the Wedderburn quasi-likelihood family

Methods and Accessor Functions	
confint.gnm	compute confidence intervals of *gnm* parameters based on the profiled deviance
confint.profile.gnm	compute confidence intervals of parameters from a *profile.gnm* object
predict.gnm	predict from a *gnm* model
profile.gnm	profile deviance for parameters in a *gnm* model
plot.profile.gnm	plot profile traces from a *profile.gnm* object
summary.gnm	summarize *gnm* fits
residSVD	multiplicative approximation of model residuals
exitInfo	print numerical details of last iteration when **gnm** has not converged
ofInterest	extract the *ofInterest* component of a *gnm* object
ofInterest<-	replace the *ofInterest* component of a *gnm* object
parameters	get model parameters from a *gnm* object, including parameters that were constrained
pickCoef	get indices of model parameters
getContrasts	estimate contrasts and their standard errors for parameters in a *gnm* model
checkEstimable	check whether one or more parameter combinations in a *gnm* model is identified
se	get standard errors of linear parameter combinations in *gnm* models
Dref	estimate weights and corresponding standard errors for a diagonal reference term in a *gnm* model
termPredictors	(*generic*) extract term contributions to predictor

Auxiliary Functions	
asGnm	coerce an object of class *lm* or *glm* to class *gnm*
expandCategorical	expand a data frame by re-expressing categorical data as counts
getModelFrame	get the model frame in use by **gnm**
MPinv	Moore-Penrose pseudoinverse of a real-valued matrix
qrSolve	Minimum-length solution of a linear system

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