# Generalized nonlinear models in R: an overview of the gnm package

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For gnm version 0.9-1, 2006-10-11

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<sup>\*</sup>This work was supported by the Economic and Social Research Council (UK) through a Professorial Fellowship.

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# 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 1m and g1m 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:

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)</pre>
```

```
> comparison1 <- anova(independence, quasi.indep, quasi.symm)</pre>
> 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
          9 125923.29
2
          5
                 69.51 4 125853.78
3
                  2.99 2
          3
                              66.52
> comparison2 <- anova(symmetry, quasi.symm)</pre>
> 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
               243.550
          6
                 2.986 3 240.564
          3
```

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  $L_1 \times ... \times L_k$ , where  $L_i$  is the number of levels for the *i*th 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):

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:

```
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:
 > ### Fit the levels models given in Table 3 of Xie (1992)
 > ## Null association between origin and destination
 > nullModel <- gnm(Freq ~ country:origin + country:destination,</pre>
                     family = poisson, data = erikson, verbose = FALSE)
 > ## Interaction specified by levelMatrix, common to all countries
 > commonTopo <- update(nullModel, ~ . +</pre>
                         Topo(origin, destination, spec = levelMatrix),
                         verbose = FALSE)
 > ## Interaction specified by levelMatrix, different multiplier for
 > ## each country
 > multTopo <- update(nullModel, ~ . +</pre>
                       Mult(Exp(country), Topo(origin, destination, spec = levelMatrix)),
                       verbose = FALSE)
 > ## Interaction specified by levelMatrix, different effects for
 > ## each country
 > separateTopo <- update(nullModel, ~ . +</pre>
                           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
                                  7.9
 4
          93
                  208.5
                           8
```

> levelMatrix <- matrix(c(2, 3, 4, 6, 5, 6, 6,

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

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))</pre>

```
col Symm(row, col)
   (Intercept)
                     row
1
   -0.2641848 0.0000000 0.000000
                                       9.62354843
    -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
    -0.2641848 4.8693457 1.539852
                                       0.07295506
    -0.2641848 4.8693457 5.082641
                                      -3.94766844
    -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
   -0.2641848 0.7465235 5.082641
                                       0.00000000
12
   -0.2641848 4.4109017 0.000000
                                       0.00000000
   -0.2641848 4.4109017 4.918310
                                      -3.94766844
   -0.2641848 4.4109017 1.539852
                                       0.00000000
                                       0.00000000
   -0.2641848 4.4109017 5.082641
```

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

```
5
                           2
                                                         4
0.000000e+00
               0.000000e+00
                              0.000000e+00
                                             0.000000e+00
                                                            0.000000e+00
                                                                          -1.776357e-15
                           8
                                          9
                                                        10
                                                                       11
-8.881784e-16 -8.881784e-16
                              0.000000e+00
                                             0.000000e+00
                                                            0.000000e+00
                                                                           0.000000e+00
           13
                          14
                                         15
                                                        16
0.000000e+00 -1.776357e-15 -8.881784e-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 nonlin functions. There are several nonlin functions in the gnm package. Some of these specify simple mathematical functions of predictors: Exp, Log, Mult, Inv, Raise (to raise to a constant power), and Logit. Others specify more specialised nonlinear terms, in particular MultHomog specifies homogeneous multiplicative interactions and Dref specifies diagonal reference terms. Users may also define their own nonlin functions.

In previous versions of gnm, specialised nonlinear terms were implemented using plug-in functions and users could define custom plug-in functions as described in Section 3.6. Such functions still work in the current version of gnm, but as plug-in functions are less user-friendly than *nonlin* functions, support for plug-in functions is likely to be withdrawn in future versions.

#### 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

Log the natural logarithm of a predictor

**Logit** the logit of a predictor

Mult the product of predictors

Raise a predictor raised to a constant power

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, one way to specify a logistic term of the form

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

would be as follows

However, this is rather convoluted and it may be preferable to define a specialised *nonlin* function in such a case. Section ?? 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 by the following formula

$$mu \sim R + C + Mult(R, C)$$

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<sup>1</sup> 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 the following formula

$$mu \sim R:T + C:T + Mult(Exp(T), R:C)$$

# 3.2 MultHomog

MultHomog is 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 mu, the formula argument to gnm would be

$$mu \sim R + C + Diag(R, C) + MultHomog(R, C)$$

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.

<sup>&</sup>lt;sup>1</sup> 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.

#### 3.3 Dref

Dref is a *nonlin* function to fit diagonal reference terms 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  $\gamma_l$  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  $\gamma_l$ , 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  $\delta_f$  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 the formula

$$mu \sim -1 + Dref(R, C)$$

The *Dref* function has one specified argument, *delta*, which is a formula with no left-hand side, specifying the dependence of  $\delta_f$  on any covariates. For example, the formula

$$mu \sim -1 + x + Dref(R, C, delta = \sim 1 + x)$$

specifies the following 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  $\delta_f$  or the  $\xi_f$ , rather than the implied weights  $w_f$ .

# 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

$$mu \sim R + C + Mult(R, C, inst = 1) + Mult(R, C, inst = 2)$$

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

$$mu \sim R + C + instances(Mult(R, C), 2)$$

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

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 with the following components:

**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 departed mathematical expression of the nonlinear term. Only functions recognised by *deriv* should be used in the expression, e.g. + rather than *sum*.

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

The list returned by the *nonlin* function should also include the following components as necessary:

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.

and may include any of the following components:

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 be matched sequentially to the arguments of *call*.

**start** an optional 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, A, A, A, A, 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).

As an example, consider the following logistic term

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

We can consider Asym, xmid and scal as the parameters of three separate predictors, each with a single intercept term. Thus our *predictors* component would be

```
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 return the following variables component

```
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). Now we need to specify a function that will paste together an expression for the term, given labels for the predictors and the variables:

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

This would be the *term* component returned by our *nonlin* function.

We now have all the necessary ingredients of a *nonlin* function to specify the logistic term. Since the parameterisation 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 specified by the labels of the *predictors* component. Since we do not anticipate fitting models with multiple logistic terms, our *nonlin* will not return a *call* component with which to prefix the parameter labels. We do however, have some idea of useful starting values, so we will specify the following *start* component

```
function(theta){
  theta[3] <- 1
  theta
}</pre>
```

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"</pre>
```

The MultHomog function provides a further example a nonlin function, showing how to specify a term with quite different features from the logistic term:

```
MultHomog <- function(..., inst = NULL){
    dots <- match.call(expand.dots = FALSE)[["..."]]
    list(predictors = dots,
        common = rep(TRUE, length(dots)),
        term = function(predLabels, ...) {
            paste("(", paste(predLabels, collapse = ")*("), ")", sep = "")
        },
        call = as.expression(match.call()),
        match = rep(0, length(dots)))
}
class(MultHomog) <- "nonlin"</pre>
```

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

The *common* component specifies that homogeneous effects are to be estimated across all the specified factors. The term only depend 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, a *call* component is returned, 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 a vector of zeros is returned as the *match* component.

# 3.6 Using Custom Plug-ins to Fit Nonlinear Terms

Prior to the introduction of *nonlin* functions, nonlinear terms that could not be specified and estimated using the in-built capability of *gnm* had to be fitted using plug-in functions. The plug-in functions previously distributed with gnm have now been implemented as *nonlin* functions, however user-specified plug-in functions may still be used with the current

version of gnm as documented in ?Nonlin. Nevertheless, support for plug-in functions is likely to be withdrawn in future versions, in favour of the simpler *nonlin* functions.

# **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 tolerance, iterStart and iterMax. Starting values for the parameter estimates can be set by start and parameters can be constrained to zero by specifying a constrain argument. 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 <code>iterStart</code> and <code>iterMax</code> 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 <code>verbose</code> or <code>trace</code> to <code>TRUE</code>. If <code>verbose</code> is <code>TRUE</code> and <code>trace</code> is <code>FALSE</code>, which is the default setting, progress is indicated by printing the character "." at the beginning of each iteration. If <code>trace</code> is <code>TRUE</code>, the deviance is printed at the beginning of each iteration (over-riding the printing of "." if necessary). Whenever <code>verbose</code> is <code>TRUE</code>, additional messages indicate each stage of the fitting process and diagnose any errors that cause that cause the algorithm to restart.

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 Using start

In some contexts, the default starting values may not be appropriate and the 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 (NAs) 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:

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.

The starting procedure used by gnm is as follows

1. Generate starting values  $\theta_i$  for all parameters  $i=1,\ldots,p$  from the Uniform(-0.1, 0.1) distribution. Shift these values away from zero as follows

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

- 2. Replace generic starting values with default starting values set by *nonlin* functions or plug-in functions, where applicable.
- 3. Replace default starting values with any starting values specified by the start argument of gnm.
- 4. Compute the *glm* estimate of any parameters that may be treated as linear (i.e. those in linear terms or those with a default starting value of *NA* set by a plug-in function), offsetting the contribution to the predictor of any fully terms specified by steps 2 and 3.

5. Run starting iterations: update one at a time any nonlinear parameters not specified by steps 2 and 3, updating *all* parameters that may be treated as linear after each round of updates.

Note that no starting iterations (step 5) will be run if all parameters are linear, or if all nonlinear parameters are specified by *start* or a plug-in function.

# 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 usually be over-parameterized and *gnm* will return a random parameterization for unidentified coefficients.

To illustrate this point, consider the following application of gnm, discussed later in Section 6.1:

Running the analysis again from a different seed

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

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)	0.0017	0.1090
origin2	0.5275	0.5198
origin3	1.6575	1.6288
origin4	2.0003	1.9510
origin5	0.7817	0.7318
origin6	2.8644	2.7965
origin7	1.5548	1.4723
origin8	1.3029	1.2118
destination2	0.9465	0.9388
destination3	2.0020	1.9732
destination4	2.2887	2.2395
destination5	1.6811	1.6312
destination6	3.1679	3.1000
destination7	2.3064	2.2239
destination8	1.8783	1.7872
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	-1.5439	1.5087
MultHomog(origin, destination)2	-1.3256	1.2905
MultHomog(origin, destination)3	-0.7275	0.6923
MultHomog(origin, destination)4	-0.1436	0.1084
MultHomog(origin, destination)5	-0.1264	0.0912
MultHomog(origin, destination)6	0.3853	-0.4205
MultHomog(origin, destination)7	0.8015	-0.8367
MultHomog(origin, destination)8	1.0451	-1.0802

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,
```

#### Deviance Residuals:

verbose = FALSE)

```
Min 1Q Median 3Q Max
-1.659e+00 -4.297e-01 -1.825e-08 3.862e-01 1.721e+00
```

#### Coefficients:

	Estimate	Std. Error	z value	Pr(> z )
(Intercept)	0.10903	NA	NA	NA
origin2	0.51978	NA	NA	NA
origin3	1.62883	NA	NA	NA
origin4	1.95104	NA	NA	NA
origin5	0.73179	NA	NA	NA
origin6	2.79654	NA	NA	NA
origin7	1.47229	NA	NA	NA
origin8	1.21183	NA	NA	NA
destination2	0.93879	NA	NA	NA
destination3	1.97324	NA	NA	NA
destination4	2.23947	NA	NA	NA
destination5	1.63121	NA	NA	NA
destination6	3.10002	NA	NA	NA
destination7	2.22389	NA	NA	NA
destination8	1.78721	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
<pre>MultHomog(origin, destination)1</pre>	1.50875	NA	NA	NA
<pre>MultHomog(origin, destination)2</pre>	1.29045	NA	NA	NA
<pre>MultHomog(origin, destination)3</pre>	0.69229	NA	NA	NA
MultHomog(origin, destination)4	0.10841	NA	NA	NA
MultHomog(origin, destination)5	0.09124	NA	NA	NA
MultHomog(origin, destination)6	-0.42052	NA	NA	NA
<pre>MultHomog(origin, destination)7</pre>	-0.83666	NA	NA	NA
MultHomog(origin, destination)8	-1.08023	NA	NA	NA

(Dispersion parameter for poisson family taken to be 1)

 $\operatorname{Std}.$  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. For example, setting the last level of the homogeneous multiplicative factor to zero,

```
> multCoef <- coef(RChomog1)[pickCoef(RChomog1, "Mult")]
> set.seed(1)
> RChomogConstrained1 <- update(RChomog1, constrain = 31, start = c(rep(NA, + 23), multCoef - multCoef[8]))
> set.seed(2)
> RChomogConstrained2 <- update(RChomogConstrained1)
> identical(coef(RChomogConstrained1), coef(RChomogConstrained2))
[1] TRUE
```

gives the same results regardless of the random seed set beforehand.

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*.

The factor to be *eliminate*-d should be specified by an expression, which is then interpreted as the first term in the model formula, replacing any intercept term. So, for example, in terms of the structure of the model,

```
gnm(mu \sim A + B + Mult(A, B), eliminate = strata1:strata2) is equivalent to gnm(mu \sim -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, unless otherwise specified through the *ofInterest* argument to *gnm*, the *ofInterest* component of the returned model object indexes the non-eliminated parameters. Thus eliminated parameters are excluded from printed model summaries and default selection by *gnm* methods. See Section 5.2 for further details on the use of the *ofInterest* component.

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 6.6 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)</pre>
```

The logistic model for dependence on x can be fitted as a Poisson log-linear model<sup>2</sup>, using either g1m or qnm:

<sup>&</sup>lt;sup>2</sup>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 *Nonlin* terms.

Here the use of *eliminate* causes the *gnm* calculations to run more quickly than *glm*. The speed advantage<sup>3</sup> increases with the number of eliminated parameters (here 1000). Since the default behaviour has not been over-ridden by an *ofInterest* argument, the eliminated parameters do not appear in printed model summaries:

```
> summary(temp.gnm)
Call:
gnm(formula = counts ~ resp + resp:x, eliminate = rowID, family = poisson,
    verbose = FALSE)
Deviance Residuals:
     Min
            10
                         Median
                                        3Q
                                                  Max
-2.852038 \quad -0.786172 \quad -0.004534
                                  0.645278
                                             2.755013
Coefficients of interest:
          Estimate Std. Error z value Pr(>|z|)
resp2
       -1.9614483 0.0340074 -57.68 <2e-16
      -1.2558460 0.0253589 -49.52
                                        <2e-16
resp3
resp1:x 0.0001049
                           NΑ
                                   NΑ
                                            NΑ
resp2:x -0.0155083
                           NA
                                   NA
                                            NA
resp3:x 0.0078314
                           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: 2462.6 on 1996 degrees of freedom
AIC: 12028
```

As usual, *gnm* has worked here with an over-parameterized representation of the model. The parameterization used by *glm* can be seen from

Number of iterations: 3

(we will not print the full summary of temp.glm here, since it gives details of all 1005 parameters!), which easily can be obtained, if required, by using getContrasts:

```
> getContrasts(temp.gnm, ofInterest(temp.gnm)[5:3])
```

<sup>&</sup>lt;sup>3</sup>In fact *eliminate* is, in principle, capable of much bigger time savings than this: its implementation in the current version of gnm is really just a proof of concept, and it has not yet been optimized for speed.

```
resp3:x 0.00000 0.00000 0.02163 0.000468
resp2:x -0.02334 0.03761 0.03077 0.000947
resp1:x -0.00773 0.02452 0.01154 0.000133
```

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 1 shows those that can be used to analyse gnm objects, whilst Figure 2 shows those that are not implemented for gnm objects.

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

Figure 1: Generic functions in the base, stats and graphics packages that can be used to analyse gnm objects.

add1	effects
alias	influence
dfbeta	kappa
dfbetas	predict
drop1	proj
dummy.coef	

Figure 2: 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.

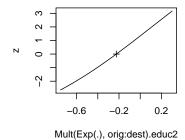
In addition to the accessor functions shown in Figure 1, the gnm package provides a new generic function called termPredictors that has methods for objects of class gnm, glm and lm. This function returns the additive contribution of each term to the predictor. See Section 2.5 for an example of its use.

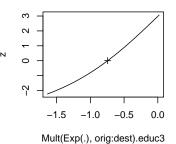
Most of the functions listed in Figure 1 can be used as they would be for *glm* or *lm* objects, however care must be taken with *vcov.gnm*, as the variance-covariance matrix will depend on the parameterization of the model. In particular, standard errors calculated using the variance-covariance matrix will only be valid for parameters or contrasts that are estimable!

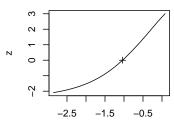
Similarly, profile.gnm and confint.gnm are only applicable to estimable parameters. The deviance function of a generalised nonlinear model can sometimes be far from quadratic and profile.gnm attempts to detect assymetry or asymptotic behaviour in order to return a sufficient profile for a given parameter. As an example, consider the following model, described later in Section 6.3:

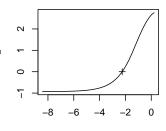
If the deviance is quadratic in a given parameter, the profile trace will be linear. We can plot the profile traces as follows:

# Profile traces for the multipliers of the orig:dest association









Mult(Exp(.), orig:dest).educ4

Mult(Exp(.), orig:dest).educ5

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).educ4. 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
- [8] 0.1053072 0.1053072 0.1053072

When the deviance is assymmetric, profile.gnm uses different stepsizes 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
- [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)

# 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. An example of this has been seen in Section 4.4, where a factor is required in the model in order to represent a structural aspect of the data, but the estimated factor effects have no substantive interpretation. Even for models in which all parameters correspond to variables of potential interest, the substantive focus may still be on a subset of parameters.

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 of Interest 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, that is described later in Section 6.3:

The effects of the first constituent multiplier in the first multiplicative interaction are identified when the estimate of one of these effects is constrained to zero, say for the effect of the first level. The parameters to be estimated are then the differences between each effect and the effect of the first level. 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)
> 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
                                                                             V
 Mult(Exp(.), religion:vote).election3
                                                                             1
                                                                             0
 Mult(Exp(.), religion:vote).election4
                                        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
                                                                        TRUE
Mult(Exp(.), religion:vote).election3 Mult(Exp(.), religion:vote).election4
                                 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))</pre>
> contrCoefs <- coefs[grep("[.]religion", coefs)]</pre>
> nContr <- length(contrCoefs)</pre>
> contrMatrix <- matrix(0, length(coefs), length(contrCoefs), dimnames = list(coefs,</pre>
      contrCoefs))
> contr <- contr.sum(contrCoefs)</pre>
> 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
Mult(Exp(election), .).religion3:vote2 Mult(Exp(election), .).religion4:vote2
                                  FALSE
                                                                            FALSE
```

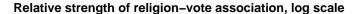
#### 5.4 getContrasts, se

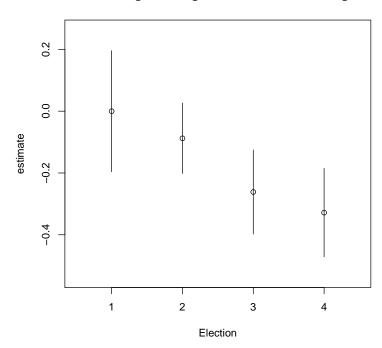
To investigate simple "sum to zero" contrasts such as those above, it is easiest to use the getContrasts function, which checks the estimability of the contrasts and returns the parameter estimates with their standard errors. Returning to the example of the first constituent multiplier in the first multiplicative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

```
> myContrasts <- getContrasts(doubleUnidiff, pickCoef(doubleUnidiff, ", religion:vote"))</pre>
> myContrasts
                                        estimate
                                                         SE
                                                               auasiSE
Mult(Exp(.), religion:vote).election1 0.0000000 0.0000000 0.09803075 0.009610029
Mult(Exp(.), religion:vote).election2 -0.0878181 0.1136832 0.05702819 0.003252214
Mult(Exp(.), religion:vote).election3 -0.2615200 0.1184134 0.06812239 0.004640660
Mult(Exp(.), religion:vote).election4 -0.3283459 0.1221302 0.07168290 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)
```





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.

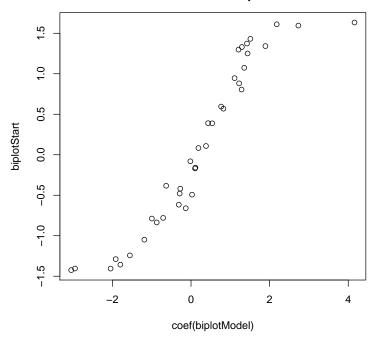
As an illustration, consider the biplot model described in Section 6.5 below. We can proceed by fitting a smaller model, then use *residSVD* to obtain starting values for the parameters in the bilinear term:

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 6.4), 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 the following plot:

# Comparison of residSVD and MLE for a 2-dimensional biplot model



# 6 Examples

This section provides some examples of the wide range of models that may be fitted using the gnm package. Sections 6.1, 6.2 and 6.3 consider various models for contingency tables; Section 6.4 considers AMMI and GAMMI models which are typically used in agricultural applications, and Section 6.6 considers the stereotype model, which is used to model an ordinal response.

# 6.1 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.

# 6.1.1 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  $\mu_{rc}$  is given by

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

We shall fit this model to the *mentalHealth* data set taken 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*:

```
> data(mentalHealth)
 > mentalHealth$MHS <- C(mentalHealth$MHS, treatment)</pre>
 > mentalHealth$SES <- C(mentalHealth$SES, treatment)</pre>
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
                                               0.03048
                   0.32802
                                                                          -0.02322
 Mult(SES, .).MHSimpaired
                  -0.27035
 Deviance:
                       3.570562
 Pearson chi-squared: 3.568088
 Residual df:
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))</pre>
 > colProbs <- with(mentalHealth, tapply(count, MHS, sum)/sum(count))</pre>
 > rowScores <- coef(RC1model)[10:15]</pre>
 > colScores <- coef(RC1model)[16:19]</pre>
 > rowScores <- rowScores - sum(rowScores * rowProbs)</pre>
 > colScores <- colScores - sum(colScores * colProbs)</pre>
 > beta1 <- sqrt(sum(rowScores^2 * rowProbs))</pre>
 > beta2 <- sqrt(sum(colScores^2 * colProbs))</pre>
```

> set.seed(1)

# 6.1.2 RC(2) model

Mult(SES, ., inst = 2).MHSimpaired

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,</pre>
      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
                         0.7102766
                                                              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
                                                             -0.0465425
                                           Mult(., MHS, inst = 2).SESA
Mult(SES, ., inst = 1).MHSimpaired
                        -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
```

#### 0.8711873

Deviance: 0.5225353 Pearson chi-squared: 0.523331

Residual df: 3

# 6.1.3 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:

origin2

#### Coefficients:

	-0.71372		0.57472
	origin3		origin4
	1.83431		2.30346
	origin5		origin6
	1.08854		3.28208
	origin7		origin8
	2.06256		1.86340
	destination2		destination3
	0.99373		2.17872
	destination4		destination5
	2.59190		1.98795
	destination6		destination7
	3.58556		2.81416
	destination8	Diag(origin,	destination)1
	2.43878		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		-1.76042
MultHomog(origin,	destination)2	MultHomog(origin,	destination)3
	-1.54213		-0.94396
MultHomog(origin,	destination)4	MultHomog(origin,	destination)5

(Intercept)

```
-0.36008 -0.34291
MultHomog(origin, destination)6 MultHomog(origin, destination)7 0.16885 0.58499
MultHomog(origin, destination)8 0.82856

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:

```
> data(occupationalStatus)
> RCheterog <- gnm(Freq ~ origin + destination + Diag(origin, destination) +
     Mult(origin, destination), family = poisson, data = occupationalStatus)
Initialising
Running start-up iterations..
Running main iterations......
> 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
```

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

# **6.2** 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)
> data(voting)
> count <- with(voting, percentage/100 * total)
> yvar <- cbind(count, voting$total - count)</pre>
```

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,</pre>
       data = voting)
 Initialising
 Running main iterations......
 > classMobility
 Call:
 gnm(formula = yvar ~ Dref(origin, destination), family = binomial,
     data = voting)
 Coefficients:
                                    Dref(., .).origin|destination1
                      (Intercept)
                         -1.34325
                                                           -0.83454
                                    Dref(., .).origin|destination3
  Dref(., .).origin|destination2
 Dref(., .).origin|destination4
                                    Dref(., .).origin|destination5
                          0.76500
                                                            1.38370
                                   Dref(origin, destination)delta2
 Dref(origin, destination)delta1
                         -0.30736
 Deviance:
                       21.22093
 Pearson chi-squared: 18.95311
 Residual df:
                       19
and the origin and destination weights can be evaluated as below
 > prop.table(exp(coef(classMobility)[2:3]))
```

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

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

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

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

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 +</pre>
      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)
                                                                       -1.32619
              Dref(., ., delta = ~ 1 + downward + upward).origin|destination1
                                                                       -0.73140
              Dref(., ., delta = ~ 1 + downward + upward).origin|destination2
              Dref(., ., delta = ~ 1 + downward + upward).origin|destination3
              Dref(., ., delta = ~ 1 + downward + upward).origin|destination4
                                                                        0.75704
              Dref(., ., delta = ~ 1 + downward + upward).origin|destination5
                                                                        1.38378
 Dref(origin, destination, delta = ~ . + downward + upward).delta1(Intercept)
                                                                        0.30662
       Dref(origin, destination, delta = ~ 1 + . + upward).delta1downwardTRUE
                                                                        0.90538
       Dref(origin, destination, delta = ~ 1 + downward + .).delta1upwardTRUE
 Dref(origin, destination, delta = ~ . + downward + upward).delta2(Intercept)
       Dref(origin, destination, delta = ~ 1 + . + upward).delta2downwardTRUE
                                                                       0.09462
       Dref(origin, destination, delta = ~ 1 + downward + .).delta2upwardTRUE
                                                                        0.53011
 Deviance:
                      18.97407
 Pearson chi-squared: 17.07493
 Residual df:
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
 > prop.table(exp(coef(socialMobility)[c(4, 7)] + coef(socialMobility)[c(2,
       5)1))
              Dref(., ., delta = ~1 + downward + upward).origin|destination3
                                                                    0.07844572
 Dref(origin, destination, delta = ~ . + downward + upward).delta1(Intercept)
                                                                    0.92155428
 > prop.table(exp(coef(socialMobility)[c(3, 6)] + coef(socialMobility)[c(2,
       5)1))
 Dref(., ., delta = ~ 1 + downward + upward).origin|destination2
                                                       0.06545295
 Dref(., ., delta = ~1 + downward + upward).origin|destination5
                                                       0.93454705
 > prop.table(exp(coef(socialMobility)[c(2, 5)]))
 Dref(., ., delta = ~1 + downward + upward).origin|destination1
```

0.8158448

Dref(., ., delta = ~ 1 + downward + upward).origin|destination4

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 groups than for the other groups. The weights for the upwardly mobile groups are very similar to the base level weights, so the model may be simplified by only fitting separate weights for the downwardly mobile groups:

```
> 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)
                                                           -1.32728
             Dref(., ., delta = ~ 1 + downward).origin|destination1
             Dref(., ., delta = ~ 1 + downward).origin|destination2
                                                            0.22076
             Dref(., ., delta = ~1 + downward).origin|destination3
                                                           -0.66437
             Dref(., ., delta = ~ 1 + downward).origin|destination4
                                                            0.75421
             Dref(., ., delta = ~1 + downward).origin|destination5
Dref(origin, destination, delta = ~ . + downward).delta1(Intercept)
      Dref(origin, destination, delta = \sim 1 + .).delta1downwardTRUE
Dref(origin, destination, delta = ~ . + downward).delta2(Intercept)
                                                            0.70439
      Dref(origin, destination, delta = ~ 1 + .).delta2downwardTRUE
                                                            0.09463
Deviance:
                     18.99389
Pearson chi-squared: 17.09981
Residual df:
> prop.table(exp(coef(downwardMobility)[c(3, 5)] + coef(downwardMobility)[c(2,
Dref(., ., delta = ~ 1 + downward).origin|destination2
                                             0.3516785
Dref(., ., delta = ~1 + downward).origin|destination4
> prop.table(exp(coef(downwardMobility)[c(2, 4)]))
Dref(., ., delta = ~ 1 + downward).origin|destination1
                                             0.4804553
Dref(., ., delta = ~1 + downward).origin|destination3
                                             0.5195447
```

# **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<sup>4</sup>, but we shall show how the models presented in the paper may be estimated using *gnm*.

<sup>&</sup>lt;sup>4</sup> We thank Frans van der Slik for his kindness in sending us the data.

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 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:

#### Coefficients:

```
MRMM
                                                                         FRMF
                    AGEM
                 0.06363
                                           -0.32425
                                                                     -0.25324
                   MWORK
                                               MFCM Dref(MOPLM, FOPLF)delta1
                -0.06430
                                           -0.06043
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
                                                                      4.43516
                 4.86458
                                            4.72343
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
                                     0.07375
                          0.06363
                                             0.863 0.38859
MRMM
                                     0.07766 -4.175 3.44e-05 ***
                         -0.32425
```

```
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
Dref(MOPLM, FOPLF)delta1 -0.33731
                                          NΑ
                                                   NΑ
                                                            NΑ
Dref(MOPLM, FOPLF)delta2 -0.02505
                                          NA
                                                   NA
                                                            NA
                                                       < 2e-16 ***
                                      0.16639
                                               29.757
Dref(., .).MOPLM|FOPLF1
                          4.95121
                                                       < 2e-16 ***
Dref(., .).MOPLM|FOPLF2
                                      0.10436
                                               46.602
                          4.86329
                                                       < 2e-16 ***
Dref(., .).MOPLM|FOPLF3
                          4.86458
                                     0.12855
                                               37.842
                                                       < 2e-16 ***
                                               34.929
Dref(., .).MOPLM|FOPLF4
                          4.72343
                                     0.13523
                                                       < 2e-16 ***
Dref(., .).MOPLM|FOPLF5
                          4.43516
                                      0.19314
                                               22.963
Dref(., .).MOPLM|FOPLF6
                                                      < 2e-16 ***
                                               24.435
                          4.18873
                                      0.17142
                                               26.231 < 2e-16 ***
Dref(., .).MOPLM|FOPLF7
                          4.43378
                                      0.16903
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
(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
```

The over-parameterization of the weights is immaterial, since the weights have been constrained to sum to one as described earlier, so the weights themselves are estimable. The weights may be evaluated as follows:

Number of iterations: 15

Dref(., .).MOPLM|FOPLF6

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$MRMM)</pre>
> FRMF2 <- as.numeric(!conformity$FRMF)</pre>
> A <- gnm(MCFM ~ -1 + AGEM + MRMM2 + FRMF2 + MWORK + MFCM +
            Dref(MOPLM, FOPLF), family = gaussian, data = conformity,
+
            verbose = FALSE)
> A
Call:
gnm(formula = MCFM \sim -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|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 \sim -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
                                                 -0.01694
Dref(MOPLM, FOPLF, delta = ~ . + MFCM).delta1(Intercept)
         Dref(MOPLM, FOPLF, delta = ~ 1 + .).delta1MFCM
Dref(MOPLM, FOPLF, delta = ~ . + MFCM).delta2(Intercept)
                                                 -0.03515
          Dref(MOPLM, FOPLF, delta = ~ 1 + .).delta2MFCM
             Dref(., ., delta = ~ 1 + MFCM).MOPLM|FOPLF1
             Dref(., ., delta = ~ 1 + MFCM).MOPLM|FOPLF2
             Dref(., ., delta = ~ 1 + MFCM).MOPLM|FOPLF3
                                                  4.83969
             Dref(., ., delta = ~ 1 + MFCM).MOPLM|FOPLF4
                                                  4.74850
             Dref(., ., delta = ~ 1 + MFCM).MOPLM|FOPLF5
             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:

giving the same weights as in Table 4 of van der Slik et al. (2002).

# 6.3 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  $\gamma_{ij}$  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)
> data(yaish)
> unidiff <- gnm(Freq ~ educ * orig + educ * dest + Mult(Exp(educ), orig:dest),</pre>
     ofInterest = "[.]educ", family = poisson, data = yaish, subset = (dest !=
Initialising
Running start-up iterations..
Running main iterations.....
Done
> coef(unidiff)
Coefficients of interest:
Mult(Exp(.), orig:dest).educ1 Mult(Exp(.), orig:dest).educ2 Mult(Exp(.), orig:dest).educ3
                  -0.5513258
                                              -0.7766976
                                                                           -1.2947494
Mult(Exp(.), orig:dest).educ4 Mult(Exp(.), orig:dest).educ5
                  -1.5902644
                                              -2.8008285
```

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 0.00000000 0.0000000 0.09757438 0.00952076
Mult(Exp(.), orig:dest).educ2 -0.2253718 0.1611874 0.12885847 0.01660450
Mult(Exp(.), orig:dest).educ3 -0.7434236 0.2335083 0.21182123 0.04486823
Mult(Exp(.), orig:dest).educ4 -1.0389386 0.3434256 0.32609380 0.10633716
Mult(Exp(.), orig:dest).educ5 -2.2495026 0.9453764 0.93560643 0.87535940
```

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)
> data(cautres)
 doubleUnidiff <- gnm(Freq ~ election * vote + election * class * religion +</pre>
      Mult(Exp(election), religion:vote) + Mult(Exp(election), class:vote),
      family = poisson, data = cautres)
Initialising
Running start-up iterations..
Running main iterations.....
> getContrasts(doubleUnidiff, rev(pickCoef(doubleUnidiff, ", religion:vote")))
                                        estimate
                                                          SE
                                                               quasiSE
Mult(Exp(.), religion:vote).election4 0.00000000 0.00000000 0.07168290 0.005138439
Mult(Exp(.), religion:vote).election3 0.06682585 0.09906916 0.06812239 0.004640660
Mult(Exp(.), religion:vote).election2 0.24052778 0.09116479 0.05702819 0.003252214
Mult(Exp(.), religion:vote).election1 0.32834589 0.12213023 0.09803075 0.009610029
> getContrasts(doubleUnidiff, rev(pickCoef(doubleUnidiff, "[.]religion")))
Mult(Exp(election), .).religion4:vote2 Mult(Exp(election), .).religion3:vote2
Mult(Exp(election), .).religion2:vote2 Mult(Exp(election), .).religion1:vote2
                                 FALSE
Mult(Exp(election), .).religion4:vote1 Mult(Exp(election), .).religion3:vote1
                                 FALSE
Mult(Exp(election), .).religion2:vote1 Mult(Exp(election), .).religion1:vote1
                                 FALSE
                                                                         FALSE
Note: not all of the specified contrasts in this set are estimable
                                       Estimate Std. Error
Mult(Exp(election), .).religion4:vote2
```

# 6.4 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  $\mu_{rc}$  a GAMMI-K model has the form

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

in which g is a link function,  $\alpha_r$  and  $\beta_c$  are the row and column main effects,  $\gamma_{kr}$  and  $\delta_{kc}$  are the row and column scores for multiplicative component k and  $\sigma_k$  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 6.1 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):

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)
Linear predictor - using glm.fit
> svdStart <- residSVD(mainEffects, year, treatment, 3)
> bilinear1 <- update(mainEffects, . ~ . + Mult(year, treatment), start = c(coef(mainEffects),
+ svdStart[, 1]))
Running main iterations
Done</pre>
```

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

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

#### 6.5 Biplot Models

Biplots are used to display two-dimensional data transformed into a space spanned by linearly independent vectors, such as the principal components or singular vectors. The plot represents the levels of the two classifying factors by their scores on the two axes which show the most information about the data, for example the first two principal components.

A rank-n model is a model based on the first n components of the decomposition. In the case of a singular value decomposition, this is equivalent to a model with n components of the multiplicative interaction.

To illustrate the use of biplot models, we shall use the *barley* data set which describes the incidence of leaf blotch over ten varieties of barley grown at nine sites (Wedderburn, 1974; Gabriel, 1998). The biplot model is fitted as follows:

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

using the *wedderburn* family function introduced in Section 2. Matrices of the row and column scores for the first two singular vectors can then be obtained by:

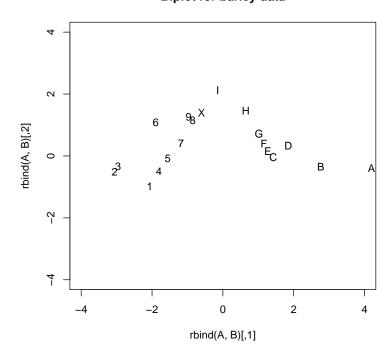
```
> barleySVD <- svd(matrix(biplotModel$predictors, 10, 9))</pre>
> A <- sweep(barleySVD$v, 2, sqrt(barleySVD$d), "*")[, 1:2]
> B <- sweep(barleySVD$u, 2, sqrt(barleySVD$d), "*")[, 1:2]
> A
            [,1]
                        [,2]
 [1,] 4.1948225 -0.39186722
 [2,] 2.7642411 -0.33951388
 [3,] 1.4250454 -0.04654266
 [4,] 1.8463067 0.33365989
 [5,]
      1.2704088 0.15776722
 [6,] 1.1562913 0.40048199
 [7,] 1.0172048 0.72727987
 [8,] 0.6451366 1.46162701
 [9,] -0.1470898 2.13234201
> B
            [,1]
                       [,2]
 [1,] -2.0673648 -0.9742045
 [2,] -3.0599797 -0.5068301
 [3,] -2.9598031 -0.3319063
 [4,] -1.8086247 -0.4975848
 [5,] -1.5579477 -0.0844451
 [6,] -1.8939995 1.0846055
 [7,] -1.1790432 0.4068701
 [8,] -0.8490092 1.1467135
```

[9,] -0.9704664 1.2655820 [10,] -0.6036789 1.3965588

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

```
> plot(rbind(A, B), pch = c(levels(barley$site), levels(barley$variety)),
+ xlim = c(-4, 4), ylim = c(-4, 4), main = "Biplot for barley data")
```

# Biplot for barley data



The product of the matrices A and B is unaffected by rotation or reciprocal scaling along either axis, so we can rotate the data so that the points for the sites are roughly parallel to the horizontal axis and the points for the varieties are roughly parallel to the vertical axis. In addition, we can scale the data so that points for the sites are about the line one unit about the horizontal axis, roughly

```
> a <- pi/5

> rotation <- matrix(c(cos(a), sin(a), -sin(a), cos(a)), 2, 2, byrow = TRUE)

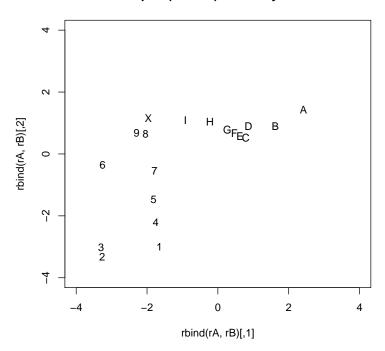
> rA <- (2 * A/3) %*% rotation

> rB <- (3 * B/2) %*% rotation

> plot(rbind(rA, rB), pch = c(levels(barley$site), levels(barley$variety)),

+ xlim = c(-4, 4), ylim = c(-4, 4), main = "Biplot (rotated) for barley data")
```

# Biplot (rotated) for barley data



In the original biplot, the co-ordinates for the sites and varieties were given by the rows of A and B respectively, i.e

$$\alpha_i^T = \sqrt{(d)}(u_{1i}, u_{2i})$$
  
 $\beta_i^T = \sqrt{(d)}(v_{1i}, v_{2i})$ 

The rotated and scaled biplot suggests the simpler model

$$\alpha_i^T = (\gamma_i, 1)$$
  
 $\beta_i^T = (\delta_j, \tau_j)$ 

which implies the following model for the logits of the leaf blotch incidence:

$$\alpha_i^T \beta_i = \gamma_i \delta_i + \tau_i.$$

Gabriel (1998) describes this as a double additive model, which we can fit as follows:

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] 9.513774 15.000000
```

# 6.6 Stereotype Model

The stereotype model was proposed by Anderson (1984) for ordered categorical data. It is a linear logistic model, in which there is assumed to be a common relationship between the response and the covariates in the model, but the scale of this association varies between categories and there is an additional category main effect or category-specific intercept:

$$\log \mu_{ic} = \beta_{0c} + \gamma_c \sum_r \beta_r x_{ir}.$$

This model can be estimated by re-expressing the categorical data as counts and using a *gnm* model with a log link and poisson variance function. The gnm package includes the utility function *expandCategorical* to facilitate the required data processing.

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. These data can be re-expressed as follows:

```
> set.seed(1)
> data(backPain)
> backPain[1:2, ]
 x1 x2 x3
                       pain
  1 1 1
  1 1 1 marked.improvement
> backPainLong <- expandCategorical(backPain, "pain")</pre>
> backPainLong[1:12, ]
   x1 x2 x3
                           pain count id
1
    1 1 1
                          worse
                                    0 1
1.1 1
       1
          1
                           same
                                    1
                                       1
1.2 1 1 1
             slight.improvement
                                       1
1.3 1 1 moderate.improvement
1.4 1 1 1
             marked.improvement
1.5 1 1 1
                 complete.relief
                                    0 1
2
    1 1 1
                          worse
                                       2
2.1 1 1 1
                                    0
                           same
                                       2
2.2 1
         1
              slight.improvement
                                    0
       1
                                       2
2.3
       1
          1 moderate.improvement
                                       2
       1
          1
              marked.improvement
                                    1
    1
       1
          1
                 complete.relief
```

We can now fit the stereotype model to these data:

```
painmoderate.improvement
                                          12.4556
                          painmarked.improvement
                                          19.9140
                             paincomplete.relief
                                          21.6653
                 Mult(., x1 + x2 + x3).painworse
                                           0.3258
                 Mult(., x1 + x2 + x3).painsame
                                          -1.8960
   Mult(., x1 + x2 + x3).painslight.improvement
 Mult(., x1 + x2 + x3).painmoderate.improvement
                                          -1.2511
   Mult(., x1 + x2 + x3).painmarked.improvement
                                          -2.4362
      Mult(., x1 + x2 + x3).paincomplete.relief
                      Mult(pain, . + x2 + x3).x1
                                           1.6697
                      Mult(pain, x1 + . + x3).x2
                                           0.9577
                      Mult(pain, x1 + x2 + .).x3
                                           0.8432
 Deviance:
                       303.1003
 Pearson chi-squared: 433.3727
 Residual df:
                       493
specifying the id factor through eliminate so that the 101 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 x = 1
(x_1, x_2, x_3). 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,</pre>
       family = "poisson", data = backPainLong)
 Initialising
 Running main iterations.....
 Done
 > threeDimensional
 gnm(formula = count \sim pain + pain:(x1 + x2 + x3), eliminate = id,
     family = "poisson", data = backPainLong)
 Coefficients of interest:
                     painsame
                                     painslight.improvement
                                                                 painmoderate.improvement
                      36.0994
                                                                                    32.6011
                                                     35.7186
      painmarked.improvement
                                        paincomplete.relief
                                                                              painworse:x1
                      39.8017
                                                     42.2498
                                                                                    10.6708
                  painsame:x1
                                  painslight.improvement:x1
                                                              painmoderate.improvement:x1
                                                     -2.5559
                      -2.8855
                                                                                    -2.2924
   painmarked.improvement:x1
                                     paincomplete.relief:x1
                                                                              painworse:x2
                                                                                    0.4189
                      -4.1156
                                                     -4.6275
                  painsame:x2
                                  painslight.improvement:x2
                                                              painmoderate.improvement:x2
                      -2.2551
                                                     -2.1325
                                                                                    -1.2531
                                                                              painworse:x3
   painmarked.improvement:x2
                                     paincomplete.relief:x2
                      -2.4249
                                                     -2.8561
                                                                                    -1.7476
```

painslight.improvement:x3 painmoderate.improvement:x3

painsame:x3

```
-2.9031 -3.0397 -2.4938
painmarked.improvement:x3 paincomplete.relief:x3
-3.4391 -4.6883

Deviance: 299.0152
Pearson chi-squared: 443.0043
Residual df: 485
```

This model has the maximum dimensionality of three (as determined by the number of covariates). To obtain the log-likelihoods as reported in Anderson (1984) we need to adjust for the extra parameters introduced to formulate the models as Poisson models. We write a simple function to do this and compare the log-likelihoods of the one dimensional model and the three dimensional model:

```
> logLikMultinom <- function(model) {</pre>
      object <- get(model)</pre>
      if (inherits(object, "gnm")) {
+
+
          1 <- logLik(object) + object$eliminate</pre>
+
          c(nParameters = attr(1, "df") - object$eliminate, logLikelihood = 1)
      else c(nParameters = object$edf, logLikelihood = -deviance(object)/2)
+ }
> t(sapply(c("oneDimensional", "threeDimensional"), logLikMultinom))
                  nParameters logLikelihood
oneDimensional
                                   -151.5501
                           12
threeDimensional
                                   -149.5076
                           20
```

which show 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:

```
> summary(oneDimensional)
Call:
gnm(formula = count \sim pain + Mult(pain, x1 + x2 + x3), eliminate = id,
    family = "poisson", data = backPainLong)
Deviance Residuals:
    Min
              1Q
                  Median
                                 30
                                          Max
                                       2.1385
-0.9708 \quad -0.6506 \quad -0.4438
                           -0.1448
Coefficients of interest:
                                                 Estimate Std. Error z value Pr(>|z|)
painsame
                                                  16.1578
                                                                   NA
                                                                            NA
                                                                                     NA
painslight.improvement
                                                  15.6848
                                                                   NA
                                                                            NA
                                                                                     NA
painmoderate.improvement
                                                  12.4556
                                                                   NA
                                                                            NA
                                                                                     NA
painmarked.improvement
                                                  19.9140
                                                                            NA
                                                                                     NA
                                                                   NA
paincomplete.relief
                                                  21.6653
                                                                   NA
                                                                            NA
                                                                                     NA
Mult(., x1 + x2 + x3).painworse
                                                   0.3258
                                                                   NA
                                                                            NA
                                                                                     NA
Mult(., x1 + x2 + x3).painsame
                                                  -1.8960
                                                                   NA
                                                                            NA
                                                                                     NA
Mult(., x1 + x2 + x3).painslight.improvement
                                                  -1.7762
                                                                   NA
                                                                            NΑ
                                                                                     NA
Mult(., x1 + x2 + x3).painmoderate.improvement
                                                  -1.2511
                                                                   NA
                                                                            NΑ
                                                                                     NA
                                                                            NA
Mult(., x1 + x2 + x3).painmarked.improvement
                                                                   NA
                                                                                     NA
                                                  -2.4362
Mult(., x1 + x2 + x3).paincomplete.relief
                                                   -2.8915
                                                                   NA
                                                                            NΑ
                                                                                     NA
Mult(pain, . + x2 + x3).x1
                                                   1.6697
                                                                   NA
                                                                            NA
                                                                                     NA
Mult(pain, x1 + . + x3).x2
                                                   0.9577
                                                                   NA
                                                                            NA
                                                                                     NA
Mult(pain, x1 + x2 + .).x3
                                                   0.8432
                                                                   NA
                                                                            NΑ
                                                                                     NΑ
```

 $\operatorname{Std}.$  Error is NA where coefficient has been constrained or is unidentified

```
Residual deviance: 303.1 on 493 degrees of freedom
AIC: 731.1
Number of iterations: 14
> oneDimensional <- gnm(count ~ pain + Mult(pain, offset(x1) + x2 + x3),</pre>
      eliminate = id, family = "poisson", data = backPainLong)
Initialising
Running start-up iterations..
Running main iterations.....
> 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
-0.9708 -0.6506 -0.4438 -0.1448
                                     2.1385
Coefficients of interest:
                                                       Estimate Std. Error z value
painsame
                                                        16.1578
                                                                    6.5742
                                                                             2.458
painslight.improvement
                                                        15.6848
                                                                    6.5274
                                                                             2.403
painmoderate.improvement
                                                        12.4556
                                                                    6.4312
                                                                              1.937
painmarked.improvement
                                                        19.9140
                                                                    6.4976
                                                                              3.065
paincomplete.relief
                                                        21.6654
                                                                    6.5571
                                                                              3.304
Mult(., x2 + x3 + offset(x1)).painworse
                                                         1.4650
                                                                        NA
                                                                                 NA
Mult(., x2 + x3 + offset(x1)).painsame
                                                        -2.2448
                                                                        NΑ
                                                                                 NΑ
Mult(., x2 + x3 + offset(x1)).painslight.improvement
                                                        -2.0447
                                                                        NA
                                                                                 NA
Mult(., x2 + x3 + offset(x1)).painmoderate.improvement -1.1680
                                                                        NA
                                                                                 NA
Mult(., x2 + x3 + offset(x1)).painmarked.improvement
                                                        -3.1466
                                                                        NA
                                                                                 NA
Mult(., x2 + x3 + offset(x1)).paincomplete.relief
                                                        -3.9069
                                                                        NA
                                                                                 NA
                                                                    0.2178
Mult(pain, . + x3 + offset(x1)).x2
                                                         0.5736
                                                                             2.633
Mult(pain, x2 + . + offset(x1)).x3
                                                                    0.2431
                                                                             2.077
                                                         0.5050
                                                       Pr(>|z|)
painsame
                                                       0.013980
painslight.improvement
                                                       0.016265
painmoderate.improvement
                                                       0.052777
painmarked.improvement
                                                       0.002178
                                                       0.000953
paincomplete.relief
Mult(., x2 + x3 + offset(x1)).painworse
                                                             NA
Mult(., x2 + x3 + offset(x1)).painsame
                                                             NA
Mult(., x2 + x3 + offset(x1)).painslight.improvement
                                                             NA
Mult(., x2 + x3 + offset(x1)).painmoderate.improvement
                                                             NA
Mult(., x2 + x3 + offset(x1)).painmarked.improvement
                                                             NΑ
Mult(., x2 + x3 + offset(x1)).paincomplete.relief
                                                             NA
                                                       0.008451
Mult(pain, . + x3 + offset(x1)).x2
                                                       0.037808
Mult(pain, x2 + . + offset(x1)).x3
(Dispersion parameter for poisson family taken to be 1)
Std. Error is NA where coefficient has been constrained or is unidentified
Residual deviance: 303.1 on 493 degrees of freedom
AIC: 731.1
```

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, "Mult.*pain"))
               Mult(., x2 + x3 + offset(x1)).painworse
                Mult(., x2 + x3 + offset(x1)).painsame
 Mult(., x2 + x3 + offset(x1)).painslight.improvement
Mult(., x2 + x3 + offset(x1)).painmoderate.improvement
 Mult(., x2 + x3 + offset(x1)).painmarked.improvement
     Mult(., x2 + x3 + offset(x1)).paincomplete.relief
                    Mult(pain, . + x3 + offset(x1)).x2
                    Mult(pain, x2 + . + offset(x1)).x3
                                                 FALSE
Note: not all of the specified contrasts in this set are estimable
                                                        estimate
                                                                       SE
                                                                            quasiSE
Mult(., x2 + x3 + offset(x1)).painworse
                                                        0.000000 0.000000 1.7797354
Mult(., x2 + x3 + offset(x1)).painsame
                                                       -3.709738 1.825568 0.4281334
Mult(., x2 + x3 + offset(x1)).painslight.improvement
                                                       -3.509697 1.791732 0.4024684
Mult(., x2 + x3 + offset(x1)).painmoderate.improvement -2.632943 1.669256 0.5518548
Mult(., x2 + x3 + offset(x1)).painmarked.improvement -4.611597 1.895240 0.3133220
                                                       -5.371854 1.999657 0.4919550
Mult(., x2 + x3 + offset(x1)).paincomplete.relief
                                                         quasiVar
Mult(., x2 + x3 + offset(x1)).painworse
                                                       3.16745802
Mult(., x2 + x3 + offset(x1)).painsame
                                                       0.18329822
Mult(., x2 + x3 + offset(x1)).painslight.improvement
                                                       0.16198084
Mult(., x2 + x3 + offset(x1)).painmoderate.improvement 0.30454368
Mult(., x2 + x3 + offset(x1)).painmarked.improvement
                                                       0.09817066
Mult(., x2 + x3 + offset(x1)).paincomplete.relief
                                                       0.24201969
```

giving the required estimates.

# 6.7 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

$$y = \alpha + \exp(\beta + \gamma x) + e \tag{1}$$

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

$$y = \alpha + \exp(\beta_1 + \gamma_1 x) + \exp(\beta_2 + \gamma_2 x) + e. \tag{2}$$

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.

#### 6.7.1 Example: single exponential decay term

Let us first construct some data from model (1). 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  $\alpha = 0$ ,  $\beta = 0$ ,  $\gamma = -0.1$ .

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  $(\alpha, \beta, \gamma)$ . 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:

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

#### 6.7.2 Example: sum of two exponentials

We can conduct a similar exercise based on the more complex model (2):

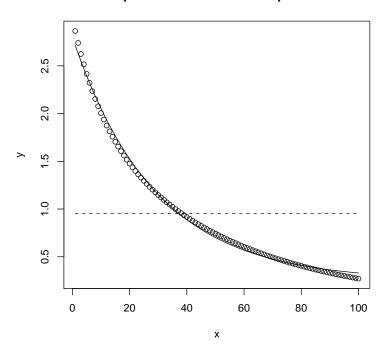
In this instance, only 14 of the 100 calls to gnm have successfully located a local maximum of the likelihood: in the remaining 86 cases the starting values generated were such that numerical problems resulted, and the fitting algorithm was abandoned (giving a NULL result). Among the 14 'successful' fits, it is evident that there are three distinct solutions (with respective residual sums of squares equal to 0.1589, 41.6, and essentially zero — the last of these, the exact fit to the data, having been found 4 times out of the above 13). 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 41.6), as we can see by comparing with:

```
> singleExp < -gnm(y \sim Exp(1 + x), start = c(NA, NA, -0.1), verbose = FALSE)
> singleExp
Call:
gnm(formula = y \sim 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)</pre>
> meanOnly
Call:
gnm(formula = y \sim 1, verbose = FALSE)
Coefficients:
(Intercept)
     0.9511
                      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")

#### Two sub-optimal fits to a sum-of-exponentials curve



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  $\gamma_1$  and  $\gamma_2$  should both be small and negative, we might perhaps have tried

(Intercept) Exp(. + x, inst = 1).(Intercept)
5.972e-08 -1.316e-08
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: 9.991902e-14
Pearson chi-squared: 9.991902e-14
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
Торо	create 'topological' interaction factors
Mult	specify a multiplicative interaction in a gnm formula
Exp	specify an exponentiated constituent multiplier in a Mult term
Nonlin	specify a special nonlinear term in a gnm formula
Dref	gnm plug-in function to fit diagonal reference terms
MultHomog	gnm plug-in function to fit multiplicative interactions with homogeneous effects
wedderburn	specify the Wedderburn quasi-likelihood family
Methods and Accessor Funct	tions
confint.gnm	compute confidence intervals of <i>gnm</i> parameters based on the profiled deviance
confint.profile.gnm	compute confidence intervals of parameters from a profile.gnm object
profile.gnm	profile deviance for parameters in a <i>gnm</i> model
plot.profile.gnm	plot profile traces from a profile.gnm object
summary.gnm	summarize <i>gnm</i> 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 <i>gnm</i> object, including parameters that were constrained
pickCoef	get indices of model parameters
getContrasts	estimate contrasts and their standard errors for parameters in a <i>gnm</i> model
checkEstimable	check whether one or more parameter combinations in a <i>gnm</i> model is identified
se	get standard errors of linear parameter combinations in <i>gnm</i> models
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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