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

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For *gnm* version 0.8-4, 2006-04-20

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^{*}This work was supported by the Economic and Social Research Council (UK) through a Professorial Fellowship.

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 lm Diag, Symm and Topo, for setting up structured interactions between factors; a new *family* function, wedderburn, for modelling a continuous response variable in [0,1] with the variance function $V(\mu) = \mu^2(1-\mu)^2$ as in Wedderburn (1974); and a new generic function termPredictors which extracts the contribution of each term to the predictor from a fitted model object. These functions are briefly introduced here, before we move on to the main purpose of the package, nonlinear models, in Section 3.

2.2 Diag and Symm

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

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

```
> count <- c(11607, 100, 366, 124, 87, 13677, 515, 302, 172, 225, + 17819, 270, 63, 176, 286, 10192)
> region <- c("NE", "MW", "S", "W")
> row <- gl(4, 4, labels = region)
> col <- gl(4, 1, length = 16, labels = region)
The comparison of models reported by Agresti can be achieved as follows:
```

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

Analysis of Deviance Table

```
Model 1: count ~ row + col
Model 2: count ~ row + col + Diag(row, col)
Model 3: count ~ row + col + Symm(row, col)
  Resid. Df Resid. Dev Df Deviance
1
             125923.29
          5
2
                 69.51 4 125853.78
3
          3
                  2.99 2
                               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
1
          6
2
          3
                 2.986
                        3
                           240.564
```

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:

```
> levelMatrix <- matrix(c(2, 3, 4, 6, 5, 6, 6,
                           3, 3, 4, 6, 4, 5, 6,
+
                           4, 4, 2, 5, 5, 5, 5,
+
                           6, 6, 5, 1, 6, 5, 2,
                           4, 4, 5, 6, 3, 4, 5,
                           5, 4, 5, 5, 3, 3, 5,
                           6, 6, 5, 3, 5, 4, 1), 7, 7, byrow = TRUE
The models of table 3 of Xie (1992) can now be fitted as follows:
> ## Null association between origin and destination
> nullModel <- gnm(Freq ~ country:origin + country:destination,</pre>
                    family = poisson, data = erikson)
Running main iterations.
Done
> ## Interaction specified by levelMatrix, common to all countries
> commonTopo <- update(nullModel, ~ . +</pre>
                        Topo(origin, destination, spec = levelMatrix))
Running main iterations.
Done
> ## Interaction specified by levelMatrix, different multiplier for each country
> multTopo <- update(nullModel, ~ . + Mult(country, Topo(origin, destination,</pre>
                                         spec = levelMatrix)))
Running start-up iterations..
Running main iterations.....
Done
> ## Interaction specified by levelMatrix, different effects for each country
> separateTopo <- update(nullModel, ~ . +</pre>
                          country:Topo(origin, destination, spec = levelMatrix))
Running main iterations.
Done
> 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
         93
                 208.5
                          8
                                 7.9
```

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

2.4 The wedderburn family

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

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

[1] 71.17401
```

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

2.5 termPredictors

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

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

> print(temp <- termPredictors(quasi.symm))</pre>

```
col Symm(row, col)
   (Intercept)
                     row
1
    -0.2641848 0.0000000 0.000000
                                       9.62354843
2
    -0.2641848 0.0000000 4.918310
                                      -0.09198126
    -0.2641848 0.0000000 1.539852
3
                                       4.63901793
    -0.2641848 0.0000000 5.082641
                                       0.00000000
5
    -0.2641848 4.8693457 0.000000
                                      -0.09198126
6
    -0.2641848 4.8693457 4.918310
                                      0.00000000
7
    -0.2641848 4.8693457 1.539852
                                      0.07295506
8
    -0.2641848 4.8693457 5.082641
                                      -3.94766844
    -0.2641848 0.7465235 0.000000
9
                                       4.63901793
10 -0.2641848 0.7465235 4.918310
                                       0.07295506
                                      7.76583039
11 -0.2641848 0.7465235 1.539852
12
    -0.2641848 0.7465235 5.082641
                                       0.00000000
    -0.2641848 4.4109017 0.000000
                                       0.00000000
   -0.2641848 4.4109017 4.918310
                                      -3.94766844
15 -0.2641848 4.4109017 1.539852
                                       0.00000000
16 -0.2641848 4.4109017 5.082641
                                       0.00000000
> rowSums(temp) - quasi.symm$linear.predictors
    2
       3
             5
                6
                  7
                      8
                         9 10 11 12 13 14 15 16
                            0
                               0
                                  0
                                     0 0
                         0
                                           0
```

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. Multiplicative interaction terms can be estimated using the in-built capability of the gnm function and are specified in the model formula using the symbolic function Mult. Other nonlinear terms can be estimated using plug-in functions for gnm and are specified using Nonlin.

There are two plug-in functions currently made available in the *gnm* package: MultHomog for fitting multiplicative interaction terms with homogeneous effects and Dref for fitting diagonal reference terms. Users of *gnm* can define their own custom plug-in functions to specify other types of nonlinear term.

3.1 Multiplicative Interaction Terms using Mult

Multiplicative interaction terms can be included in the formula argument to gnm by using the symbolic wrapper function Mult. Constituent multipliers in the interaction are passed as unspecified arguments to Mult and are expressed by symbolic linear formulae. An intercept is automatically added to each constituent multiplier unless otherwise specified. For example, to fit 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), the formula argument of gnm would be

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

where R and C are row and column factors respectively.

Mult has one specified argument *multiplicity*, which is 1 by default. This argument determines the number of times that the specified multiplicative structure appears in the model. For example,

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

would give the RC(2) model (Goodman, 1979)

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

In some contexts, it may be desirable to constrain one or more of the constituent multipliers so that it is always 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)

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

Exponentiated constituent multipliers are specified in *gnm* models using the symbolic function Exp; for example, the uniform difference model above would be specified by the formula

$$mu \sim R:T + C:T + Mult(Exp(-1 + T), R:C)$$

3.2 Other Nonlinear Terms using Nonlin

Nonlinear terms which can not be specified using Mult may be specified using Nonlin. This symbolic function indicates a term which requires a plug-in function to estimate the associated parameters. Nonlin takes a single argument, which is a call to the relevant plug-in function.

For example, in the formula

$$mu \sim x + A + B + Nonlin(PlugInFunction(A, B, arg1 = x, arg2 = C))$$

the call to Nonlin is used to specify a term that requires the plug-in function PlugInFunction.

The two plug-in functions already included in the *gnm* package are described below, followed by a guide to writing custom plug-in functions.

3.2.1 MultHomog

The MultHomog function provides the tools required to fit multiplicative interaction terms with one component 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

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.

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

3.2.2 Dref

Dref is a plug-in 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 γ_l is the "diagonal effect" for level l.

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

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

and estimating the δ_f .

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

Dref has one specified argument, *formula*, which is a symbolic description of the dependence of δ_f on any covariates. For example, the formula

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

specifies the following diagonal reference model

$$\mu_{rc} = \beta_X x + \frac{e^{\xi_1 + \beta_1 x}}{e^{\xi_1 + \beta_1 x} + e^{\xi_2 + \beta_2 x}} \gamma_r + \frac{e^{\xi_2 + \beta_2 x}}{e^{\xi_1 + \beta_x} + e^{\xi_2 + \beta_2 x}} \gamma_c.$$

The default value of *formula* is ~1, so that constant weights are estimated. The coefficients returned by gnm are those that are directly estimated, i.e. the δ_f or the ξ_f and β_f , rather than the implied weights w_f .

3.2.3 Custom Plug-in Functions

Custom plug-in functions may be written to enable gnm to fit nonlinear terms that can not be specified by Mult or through existing plug-in functions provided by the *gnm* package.

There are no constraints on the arguments that a plug-in function may take. However it is important that Nonlin, when given a call to the plug-in function, can determine the variables that are in the term, so that these variables can be added to the model frame. By default, expressions passed to unspecified arguments of the plug-in function are assumed to represent the variables in the term.

If the default action of Nonlin will not capture the required variables, a companion function must exist (in the environment of the plug-in function), which takes the same arguments as the plug-in function and returns deparsed expressions representing the necessary variables. The name of this function must be the name of the plug-in function suffixed with "Variables". For example, the (non-visible) companion function for Dref is defined as

```
DrefVariables <- function(..., formula = ~ 1) {
    as.character(c(match.call(expand.dots = FALSE)[[2]], formula[[2]]))
}</pre>
```

returning the expressions passed to unspecified arguments and the right-hand side of the formula passed to *formula*, as character strings. For instance

```
> gnm:::DrefVariables(A, B, formula = ~1 + C)
```

from which Nonlin will know that A, B and C need to be added to the model frame.

The call to the plug-in function is evaluated in the environment of the model frame and in the enclosing environment of the parent frame of the call to gnm. This should ensure that variables passed directly to the plug-in function can be found. However, to evaluate variables within the plug-in function, it may be necessary to access the model frame, which can be obtained using the function getModelFrame.

For example, the factors in a Dref term are passed directly to unspecified arguments, so the dummy variables for these factors can be found as follows:

```
# get design matrices for Dref factors
designList <- lapply(list(...), class.ind)</pre>
```

But any covariates on which the weights depend are only represented symbolically in the *formula* argument, so the design matrix for these variables must be found in the context of the model frame:

```
## get design matrix for local structure
gnmData <- getModelFrame()
local <- model.matrix(formula, data = gnmData)</pre>
```

The plug-in function should return a list with at least the following three components:

labels a character vector of labels for the parameters (to which gnm will prefix the call to the plug-in function).

predictor a function which takes a vector of parameter estimates and returns either a vector of fitted values or a matrix whose columns are additive components of the fitted values.

localDesignFunction a function which takes the specified arguments *coef* (a vector of parameter estimates) and *predictor* (the result of the predictor function), and returns the local design matrix. If the plug-in function does not return a start component (see below), the localDesignFunction must also take the argument *ind*, which specifies the index of a column to be returned instead of the full matrix.

and optionally one further component,

start a vector of default starting values for the parameters. NA may be used to indicate parameters which may be treated as linear for the purpose of finding starting values, given the non-NA values. See Section 4.2 for details of how these starting values will be used if provided and the starting procedure for nonlinear parameters that will be used otherwise.

As an example of a start component, Dref returns

```
c(runif(nLocal) - 0.5, rep(0.5, nGlobal))
```

where nLocal is the number of weight parameters (parameters which are "local" to a specific factor) and nGlobal is the number of diagonal effects ("global" level effects across factors). The randomness in the starting values for the weight parameters ensures that arbitrariness of the final parameterization is emphasised.

The ${\tt MultHomog}$ function provides a simple example of a ${\tt predictor}$ component:

```
predictor <- function(coef) {
    do.call("pprod", lapply(designList, "%*%", coef))
}</pre>
```

which computes the product of the vectors found by multiplying the design matrix for each factor in the interaction (held in designList) by the homogeneous coefficients (in coef). This function takes advantage of *lexical scoping*: designList is an object defined in MultHomog, which predictor is able to find because predictor is also defined in MultHomog and hence MultHomog is the enclosing environment of predictor.

The localDesignFunction created by MultHomog is slightly more complicated:

```
localDesignFunction <- function(coef, ind = NULL, ...) {
    X <- 0
    vList <- lapply(designList, "%*%", coef)
    for (i in seq(designList)) {
        if (is.null(ind))</pre>
```

Since the result of the predictor function is not needed here, the local design function does not have the specified argument *predictor*, but allows such an argument to be passed to the function by the use of the special argument '...'. Since MultHomog does not return a start component, the local design function can optionally return a single column of the local design matrix as specified by *ind*. This functionality is required by the default starting procedure for nonlinear parameters.

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

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 θ_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 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 terms specified by *start* or a plug-in function.
- 5. Run starting iterations: update one at a time any remaining nonlinear parameters not specified by *start* or a plug-in function, 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 <- eval(RChomog1$call)</pre>
```

gives a different representation of the same model:

```
> compareCoef <- cbind(coef(RChomog1), coef(RChomog2))
> colnames(compareCoef) <- c("RChomog1", "RChomog2")</pre>
```

> round(compareCoef, 4)

RChomog1	RChomog2
-0.1304	0.1844
0.5367	0.5143
1.6920	1.6083
2.0594	1.9158
0.8415	0.6961
2.9458	2.7480
1.6538	1.4132
1.4122	1.1466
0.9557	0.9333
2.0364	1.9527
2.3478	2.2042
1.7409	1.5955
3.2493	3.0514
2.4054	2.1648
1.9875	1.7220
	0.5367 1.6920 2.0594 0.8415 2.9458 1.6538 1.4122 0.9557 2.0364 2.3478 1.7409 3.2493 2.4054

```
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
                                  -1.5861
MultHomog(origin, destination).1
                                            -1.4836
MultHomog(origin, destination).2
                                  -1.3678
                                            -1.2653
MultHomog(origin, destination).3
                                  -0.7697
                                            -0.6671
MultHomog(origin, destination).4
                                  -0.1858
                                            -0.0832
MultHomog(origin, destination).5
                                  -0.1686
                                            -0.0661
MultHomog(origin, destination).6
                                    0.3431
                                             0.4457
MultHomog(origin, destination).7
                                    0.7593
                                             0.8618
MultHomog(origin, destination).8
                                    1.0029
                                             1.1054
```

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) +
Nonlin(MultHomog(origin, destination)), family = poisson,
data = occupationalStatus, verbose = FALSE)
```

Deviance Residuals:

```
Min 1Q Median 3Q Max
-1.6588 -0.4297 0.0000 0.3862 1.7208
```

Coefficients:

		Estimate	Std. Error	z value	Pr(> z)
(Intercept)		0.18438	NA	NA	NA
origin2		0.51428	NA	NA	NA
origin3		1.60827	NA	NA	NA
origin4		1.91578	NA	NA	NA
origin5		0.69610	NA	NA	NA
origin6		2.74796	NA	NA	NA
origin7		1.41323	NA	NA	NA
origin8		1.14664	NA	NA	NA
destination2		0.93329	NA	NA	NA
destination3		1.95268	NA	NA	NA
destination4		2.20421	NA	NA	NA
${\tt destination5}$		1.59551	NA	NA	NA
destination6		3.05143	NA	NA	NA
destination7		2.16483	NA	NA	NA
destination8		1.72201	NA	NA	NA
Diag(origin,	destination)1	1.52667	0.44658	3.419	0.00063
Diag(origin,	destination)2	0.45600	0.34595	1.318	0.18747
Diag(origin,	destination)3	-0.01598	0.18098	-0.088	0.92965
Diag(origin,	destination)4	0.38918	0.12748	3.053	0.00227
Diag(origin,	destination)5	0.73852	0.23329	3.166	0.00155

```
Diag(origin, destination)6
                                   0.13474
                                              0.07934
                                                         1.698
                                                                0.08945
Diag(origin, destination)7
                                   0.45764
                                              0.15103
                                                         3.030
                                                                0.00245
Diag(origin, destination)8
                                   0.38847
                                              0.22172
                                                         1.752
                                                                0.07976
MultHomog(origin, destination).1 -1.48357
                                                   NA
                                                            NA
                                                                     NA
MultHomog(origin, destination).2 -1.26527
                                                   NA
                                                            NA
                                                                     NA
MultHomog(origin, destination).3 -0.66711
                                                   NA
                                                            NA
                                                                     NA
MultHomog(origin, destination).4 -0.08323
                                                   NA
                                                            NA
                                                                     NA
MultHomog(origin, destination).5 -0.06606
                                                   NΑ
                                                                     NΑ
                                                            NA
MultHomog(origin, destination).6
                                                   NA
                                                            NA
                                                                     NA
                                  0.44570
MultHomog(origin, destination).7
                                  0.86184
                                                   NA
                                                            NA
                                                                     NA
MultHomog(origin, destination).8 1.10541
                                                   NΑ
                                                            NΑ
                                                                     NΑ
```

(Dispersion parameter for poisson family taken to be 1)

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

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

Number of iterations: 7

Additional constraints may be specified through the *constrain* argument of gnm. This argument indicates parameters that are to be constrained to zero in the fitting process. Parameters can be indicated by a logical vector, a numeric vector of indices, a character vector of names or, if constrain = "pick" they can be selected through a Tk dialog.

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)[grep("Mult", names(coef(RChomog1)))]
> set.seed(1)
> RChomogConstrained1 <- update(RChomog1, constrain = 31, start = c(rep(NA, 23), multCoef - multCoef[8]))
> set.seed(2)
> RChomogConstrained2 <- eval(RChomogConstrained1$call)
> 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, the simple constraints imposed by *constrain* are often sufficient to make particular 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*

Sometimes a model will include a "stratification" factor which identifies units for which a unit-specific intercept should be estimated. It is often the case that such factors have a large number of levels and though they are required in the model, are not of direct interest in themselves.

The *eliminate* argument of gnm can be used to specify a stratification factor in a model, so that this factor can be handled more efficiently. The factor should be specified by an expression, which is interpreted as the first term in the model formula, replacing any intercept term. So 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 stratification 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, the eliminated parameters are excluded from summaries of the model so that the focus is on the coefficients of interest.

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: 500 randomly-generated trinomial responses, and a single predictor variable (whose effect on the data generation is null):

```
> set.seed(1)
> n <- 500
> x \leftarrow rep(rnorm(n), rep(3, n))
> counts <- as.vector(rmultinom(n, 10, c(0.7, 0.1, 0.2)))</pre>
> rowID <- factor(rep(1:n, rep(3, n)))</pre>
> resp <- factor(rep(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 qlm or qnm:
> system.time(temp.glm <- glm(counts ~ rowID + resp + resp:x, family = poisson))</pre>
[1] 10.05 0.17 14.30 0.00 0.00
> system.time(temp.gnm <- gnm(counts ~ resp + resp:x, eliminate = rowID,
       family = poisson))
Initialising
Running main iterations...
Done
[1] 6.24 0.30 7.75 0.00 0.00
> c(deviance(temp.glm), deviance(temp.gnm))
[1] 1196.341 1196.341
Here the use of eliminate causes the gnm calculations to run more quickly than glm. The speed advantage<sup>3</sup> increases with
```

Here the use of *eliminate* causes the gnm calculations to run more quickly than glm. The speed advantage³ increases with the number of eliminated parameters (here 500). The eliminated parameters do not appear in printed model summaries:

```
> summary(temp.gnm)
Call:
gnm(formula = counts ~ resp + resp:x, eliminate = rowID, family = poisson)
Deviance Residuals:
```

```
Min 1Q Median 3Q Max -2.266771 -0.766713 -0.001797 0.375404 2.854789
```

Coefficients of interest:

```
Estimate Std. Error z value Pr(>|z|)
        -1.964709
                     0.047995
                               -40.94
                                         <2e-16
resp2
resp3
        -1.290139
                     0.036258
                               -35.58
                                         <2e-16
resp1:x -0.009198
                           NA
                                   NΑ
                                             NΑ
resp2:x -0.017474
                                             NA
                           NA
                                   NΑ
```

²For 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.

³In 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 0.045449 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: 1196.3 on 996 degrees of freedom
```

AIC: 5982.5

Number of iterations: 3

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

```
> coef(temp.glm)[-(1:500)]
```

```
resp2 resp3 resp1:x resp2:x resp3:x
-1.96470932 -1.29013922 -0.05464657 -0.06292256 NA
```

(we will not print the full summary of temp.glm here, since it gives details of all 505 parameters!), which easily can be obtained, if required, by using getContrasts:

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.

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

Figure 1: Generic functions in the base, stats and graphics packages that can be used to analyse 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 for an example of its use.

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

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.

Most of the methods listed in Figure 1 can be used as they would be for *glm* or *lm* objects, however care must be taken with *vcov*, 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!

5.2 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))</pre>
> contrCoefs <- coefs[grep("Mult1.Factor1", coefs)]</pre>
> nContr <- length(contrCoefs)</pre>
> contrMatrix <- matrix(0, length(coefs), nContr, dimnames = list(coefs,
      contrCoefs))
> contr <- contr.sum(contrCoefs)</pre>
> contr <- rbind(contr[nContr, ], contr[-nContr, ])</pre>
> contrMatrix[contrCoefs, 2:nContr] <- contr</pre>
> contrMatrix[contrCoefs, 2:nContr]
                         Mult1.Factor1.election2 Mult1.Factor1.election3
Mult1.Factor1.election1
                                                -1
Mult1.Factor1.election2
                                                 1
                                                                           0
Mult1.Factor1.election3
                                                 0
                                                                           1
Mult1.Factor1.election4
                                                                           0
                         Mult1.Factor1.election4
Mult1.Factor1.election1
                                                -1
Mult1.Factor1.election2
                                                 0
Mult1.Factor1.election3
                                                 0
Mult1.Factor1.election4
                                                 1
```

Then their estimability can be checked using checkEstimable

> checkEstimable(doubleUnidiff, contrMatrix)

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:

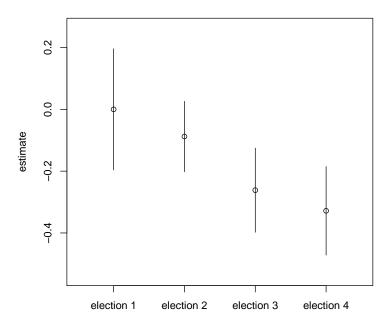
```
> coefs <- names(coef(doubleUnidiff))</pre>
> contrCoefs <- coefs[grep("Mult1.Factor2", coefs)]</pre>
> nContr <- length(contrCoefs)</pre>
> contrMatrix <- matrix(0, length(coefs), length(contrCoefs), dimnames = list(coefs,
      contrCoefs))
> contr <- contr.sum(contrCoefs)</pre>
> contrMatrix[contrCoefs, 2:nContr] <- rbind(contr[nContr, ], contr[-nContr,
> checkEstimable(doubleUnidiff, contrMatrix)
Mult1.Factor2.religion1:vote1 Mult1.Factor2.religion2:vote1
Mult1.Factor2.religion3:vote1 Mult1.Factor2.religion4:vote1
                         FALSE
Mult1.Factor2.religion1:vote2 Mult1.Factor2.religion2:vote2
                         FALSE
Mult1.Factor2.religion3:vote2 Mult1.Factor2.religion4:vote2
                         FALSE
                                                        FALSE
```

5.3 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:

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

Relative strength of religion-vote association, log scale



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.

5.4 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*.

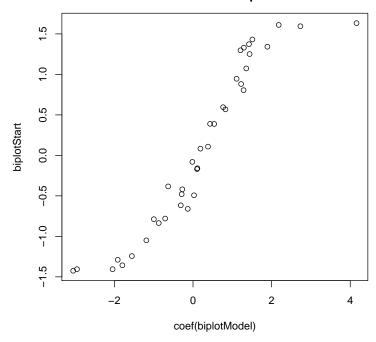
The residSVD function facilitates one particular residual analysis that is often useful when considering multiplicative interaction between factors as a model elaboration: in effect, residSVD provides a direct estimate of the parameters of such an interaction, by performing an appropriately weighted 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 μ_{rc} is given by

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

We shall fit this model to the mentalHealth data set 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":

> set.seed(1)
> data(mentalHealth)
> mentalHealth\$MHS <- C(mentalHealth\$MHS, treatment)
> 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(-1 + SES, -1 + MHS),</pre>
      family = poisson, data = mentalHealth)
Initialising
Running start-up iterations..
Running main iterations.....
Done
> RC1model
Call:
gnm(formula = count \sim SES + MHS + Mult(-1 + SES, -1 + MHS), family = poisson,
    data = mentalHealth)
Coefficients:
                                                    SESB
               (Intercept)
                  3.831281
                                              -0.067413
                      SESC
                                                    SESD
                  0.109959
                                               0.404969
                      SESE
                                                    SESF
                  0.025257
                                              -0.200685
                   MHSmild
                                            MHSmoderate
                  0.712969
                                               0.204987
                                    Mult1.Factor1.SESA
               MHSimpaired
                  0.251749
                                               0.340495
       Mult1.Factor1.SESB
                                    Mult1.Factor1.SESC
                  0.343267
                                               0.114885
       Mult1.Factor1.SESD
                                    Mult1.Factor1.SESE
                 -0.006284
                                              -0.305574
       Mult1.Factor1.SESF
                                 Mult1.Factor2.MHSwell
                 -0.551460
                                               0.935600
    Mult1.Factor2.MHSmild Mult1.Factor2.MHSmoderate
                  0.094793
                                              -0.056941
Mult1.Factor2.MHSimpaired
                 -0.755299
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>
```

> assoc <- list(beta = beta1 * beta2, mu = rowScores/beta1, nu = colScores/beta2)</pre>

> beta2 <- sqrt(sum(colScores^2 * colProbs))</pre>

> assoc

```
$beta
```

[1] 0.1664874

\$m11

\$nu

6.1.2 RC(2) model

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

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

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

```
> RC2model <- gnm(count ~ SES + MHS + Mult(-1 + SES, -1 + MHS,
+ multiplicity = 2), family = poisson, data = mentalHealth)</pre>
```

Initialising

Running start-up iterations..

Running main iterations.....

Done

> RC2model

Call:

```
gnm(formula = count ~ SES + MHS + Mult(-1 + SES, -1 + MHS, multiplicity = 2),
    family = poisson, data = mentalHealth)
```

Coefficients:

(Intercept)	SESB
3.85530	-0.06444
SESC	SESD
0.11140	0.38457
SESE	SESF
0.01081	-0.18462
MHSmild	MHSmoderate
0.69860	0.16975
MHSimpaired	Mult1.Factor1.SESA
0.22876	0.95047
Mult1.Factor1.SESB	Mult1.Factor1.SESC
0.99597	0.33932
Mult1.Factor1.SESD	Mult1.Factor1.SESE
-0.17292	-0.91634
Mult1.Factor1.SESF	Mult1.Factor2.MHSwell
-1.39376	0.35782

```
Mult1.Factor2.MHSmild Mult1.Factor2.MHSmoderate
                  0.03795
                                            -0.02129
Mult1.Factor2.MHSimpaired
                                  Mult2.Factor1.SESA
                 -0.28029
                                            -0.17762
       Mult2.Factor1.SESB
                                  Mult2.Factor1.SESC
                 -0.25156
                                            -0.16614
       Mult2.Factor1.SESD
                                  Mult2.Factor1.SESE
                  0.28993
                                             0.22675
                               Mult2.Factor2.MHSwell
       Mult2.Factor1.SESF
                 -0.45554
                                              0.30776
    Mult2.Factor2.MHSmild Mult2.Factor2.MHSmoderate
                  0.09804
                                            -0.25536
Mult2.Factor2.MHSimpaired
                  0.06769
```

0.5225353 Deviance: Pearson chi-squared: 0.523331

Residual df:

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 occupational Status 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:

```
> data(occupationalStatus)
> RChomog <- gnm(Freq ~ origin + destination + Diag(origin, destination) +
      Nonlin(MultHomog(origin, destination)), family = poisson,
      data = occupationalStatus)
Initialising
Running start-up iterations..
Running main iterations......
Done
> RChomog
Call:
```

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

Coefficients:

(Intercept)	origin2
-0.66871	0.57191
origin3	origin4
1.82383	2.28549
origin5	origin6
1.07035	3.25732
origin7	origin8

```
2.03247
                                                             1.83018
                                                        destination3
                    destination2
                          0.99093
                                                             2.16824
                    destination4
                                                        destination5
                          2.57393
                                                             1.96977
                    destination6
                                                        destination7
                          3.56080
                                                             2.78406
                                         Diag(origin, destination)1
                    destination8
                          2.40556
                                                             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
                                                             0.45764
                          0.13474
      Diag(origin, destination)8
                                   MultHomog(origin, destination).1
                          0.38847
                                                            -1.74759
MultHomog(origin, destination).2
                                   MultHomog(origin, destination).3
                         -1.52929
                                                            -0.93113
MultHomog(origin, destination).4
                                   MultHomog(origin, destination).5
                         -0.34725
                                                            -0.33008
MultHomog(origin, destination).6
                                   MultHomog(origin, destination).7
                          0.18168
                                                             0.59782
MultHomog(origin, destination).8
                          0.84139
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.....
Done
> RChomog$dev - RCheterog$dev

[1] 3.411823
> RChomog$df.residual - RCheterog$df.residual

[1] 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 3.2.2 for more detail on the parameterization.

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

```
> classMobility <- gnm(yvar ~ Nonlin(Dref(origin, destination)),
+ family = binomial, data = voting)
Initialising
Running main iterations......
Done
> classMobility
Call:
```

```
gnm(formula = yvar ~ Nonlin(Dref(origin, destination)), family = binomial,
    data = voting)
```

Coefficients:

```
(Intercept)
                                            Dref(origin, destination).origin
                             -1.34325
                                                                     -0.30736
Dref(origin, destination).destination
                                                  Dref(origin, destination).1
                             -0.05501
                                                                     -0.83455
          Dref(origin, destination).2
                                                  Dref(origin, destination).3
                              0.21066
                                                                     -0.61159
          Dref(origin, destination).4
                                                  Dref(origin, destination).5
                              0.76500
                                                                      1.38370
```

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

and the origin and destination weights can be evaluated as below

> prop.table(exp(coef(classMobility)[2:3]))

```
Dref(origin, destination).origin Dref(origin, destination).destination
0.4372469 0.5627531
```

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)
> 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 ~ Nonlin(Dref(origin, destination,
+ formula = ~1 + downward + upward)), family = binomial, data = voting)</pre>
```

Initialising

Running main iterations.....

Done

> socialMobility

Call:

Coefficients:

```
(Intercept)
                                                                                -1.31739
      Dref(origin, destination, formula = ~1 + downward + upward).origin.(Intercept)
     Dref(origin, destination, formula = ~1 + downward + upward).origin.downwardTRUE
                                                                                 0.37858
       Dref(origin, destination, formula = ~1 + downward + upward).origin.upwardTRUE
 Dref(origin, destination, formula = \sim 1 + downward + upward).destination.(Intercept)
                                                                                -0.01158
Dref(origin, destination, formula = ~1 + downward + upward).destination.downwardTRUE
                                                                                -0.43218
 Dref(origin, destination, formula = ~1 + downward + upward).destination.upwardTRUE
                                                                                 0.12247
                        Dref(origin, destination, formula = \sim 1 + downward + upward).1
                                                                                -0.74021
                        Dref(origin, destination, formula = \sim1 + downward + upward).2
                                                                                 0.20469
                        Dref(origin, destination, formula = \sim1 + downward + upward).3
                                                                                -0.67740
                        Dref(origin, destination, formula = \sim 1 + \text{downward} + \text{upward}).4
                                                                                 0.74824
                        Dref(origin, destination, formula = \sim1 + downward + upward).5
```

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

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

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:

```
Dref(origin, destination, formula = ~1 + downward).destination.(Intercept)
Dref(origin, destination, formula = \sim 1 + downward).destination.downwardTRUE
                                                                      -0.43540
                        Dref(origin, destination, formula = \sim 1 + downward).1
                       Dref(origin, destination, formula = \sim1 + downward).2
                                                                       0.20093
                        Dref(origin, destination, formula = \sim 1 + downward).3
                                                                      -0.68419
                        Dref(origin, destination, formula = \sim 1 + downward).4
                                                                      0.73438
                        Dref(origin, destination, formula = \sim 1 + downward).5
Deviance:
                     18.99389
Pearson chi-squared: 17.09981
Residual df:
> prop.table(exp(coef(downwardMobility)[c(3, 5)] + coef(downwardMobility)[c(2,
      4)]))
     Dref(origin, destination, formula = ~1 + downward).origin.downwardTRUE
                                                                    0.5991571
Dref(origin, destination, formula = ~1 + downward).destination.downwardTRUE
                                                                    0.4008429
> prop.table(exp(coef(downwardMobility)[c(2, 4)]))
     Dref(origin, destination, formula = ~1 + downward).origin.(Intercept)
                                                                   0.3992031
```

Dref(origin, destination, formula = ~1 + downward).destination.(Intercept)

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 available⁴, but we shall show how the models presented in the paper may be estimated using gnm.

0.6007969

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

$$\mu_{rc} = \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \beta_5 x_5 + \frac{e^{\delta_1}}{e^{\delta_1} + e^{\delta_2}} \gamma_r + \frac{e^{\delta_2}}{e^{\delta_1} + e^{\delta_2}} \gamma_c.$$

The baseline model can be fitted as follows:

⁴ We thank Frans van der Slik for his kindness in sending us the data.

Call:

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

Coefficients:

AGEM	MRMM	FRMF
0.06364	-0.32425	-0.25324
MWORK	MFCM	<pre>Dref(MOPLM, FOPLF).MOPLM</pre>
-0.06430	-0.06043	-0.33730
<pre>Dref(MOPLM, FOPLF).FOPLF</pre>	<pre>Dref(MOPLM, FOPLF).1</pre>	<pre>Dref(MOPLM, FOPLF).2</pre>
-0.02507	4.95123	4.86328
<pre>Dref(MOPLM, FOPLF).3</pre>	<pre>Dref(MOPLM, FOPLF).4</pre>	<pre>Dref(MOPLM, FOPLF).5</pre>
4.86458	4.72343	4.43516
<pre>Dref(MOPLM, FOPLF).6</pre>	<pre>Dref(MOPLM, FOPLF).7</pre>	
4.18873	4.43379	

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

Deviance Residuals:

```
Min 1Q Median 3Q Max -3.63689 -0.50383 0.01714 0.56752 2.25140
```

Coefficients:

		Estimate	Std. Error	t value	Pr(> t)
AGEM		0.06364	0.07375	0.863	0.38859
MRMM		-0.32425	0.07766	-4.175	3.44e-05
FRMF		-0.25324	0.07681	-3.297	0.00104
MWORK		-0.06430	0.07431	-0.865	0.38727
MFCM		-0.06043	0.07123	-0.848	0.39663
<pre>Dref(MOPLM,</pre>	FOPLF).MOPLM	-0.33730	NA	NA	NA
<pre>Dref(MOPLM,</pre>	FOPLF).FOPLF	-0.02507	NA	NA	NA
<pre>Dref(MOPLM,</pre>	FOPLF).1	4.95123	0.16639	29.757	< 2e-16
<pre>Dref(MOPLM,</pre>	FOPLF).2	4.86328	0.10436	46.601	< 2e-16
<pre>Dref(MOPLM,</pre>	FOPLF).3	4.86458	0.12855	37.842	< 2e-16
<pre>Dref(MOPLM,</pre>	FOPLF).4	4.72343	0.13523	34.928	< 2e-16
<pre>Dref(MOPLM,</pre>	FOPLF).5	4.43516	0.19315	22.963	< 2e-16
<pre>Dref(MOPLM,</pre>	FOPLF).6	4.18873	0.17142	24.435	< 2e-16
Dref(MOPLM,	FOPLF).7	4.43379	0.16903	26.231	< 2e-16

(Dispersion parameter for gaussian family taken to be 0.7384355)

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

Residual deviance: 425.34 on 576 degrees of freedom

AIC: 1507.8

Number of iterations: 10

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:

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:

Coefficients:

AGEM	MRMM2	FRMF2
0.06364	0.32425	0.25324
MWORK	MFCM	<pre>Dref(MOPLM, FOPLF).MOPLM</pre>
-0.06430	-0.06043	-0.08270
<pre>Dref(MOPLM, FOPLF).FOPLF</pre>	<pre>Dref(MOPLM, FOPLF).1</pre>	<pre>Dref(MOPLM, FOPLF).2</pre>
0.22955	4.37372	4.28579
<pre>Dref(MOPLM, FOPLF).3</pre>	<pre>Dref(MOPLM, FOPLF).4</pre>	<pre>Dref(MOPLM, FOPLF).5</pre>
4.28708	4.14593	3.85766
Dref(MOPLM, FOPLF).6	<pre>Dref(MOPLM, FOPLF).7</pre>	
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:

$$\mu_{rc} = \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \beta_5 x_5 + \frac{e^{\xi_1 + \beta_1 x}}{e^{\xi_1 + \beta_1 x} + e^{\xi_2 + \beta_2 x}} \gamma_r + \frac{e^{\xi_2 + \beta_2 x}}{e^{\xi_1 + \beta_1 x} + e^{\xi_2 + \beta_2 x}} \gamma_c.$$

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),

Coefficients:

```
AGEM
                                                   0.05818
                                                      MRMM
                                                  -0.32701
                                                      FRMF
                                                  -0.25772
                                                     MWORK
                                                  -0.07847
                                                      MFCM
                                                  -0.01694
Dref(MOPLM, FOPLF, formula = ~1 + MFCM).MOPLM.(Intercept)
                                                   0.79413
       Dref(MOPLM, FOPLF, formula = ~1 + MFCM).MOPLM.MFCM
                                                  -2.51751
Dref(MOPLM, FOPLF, formula = ~1 + MFCM).FOPLF.(Intercept)
                                                  -0.27618
       Dref(MOPLM, FOPLF, formula = ~1 + MFCM).FOPLF.MFCM
                                                   2.03673
                Dref(MOPLM, FOPLF, formula = ~1 + MFCM).1
                                                   4.82477
                Dref(MOPLM, FOPLF, formula = ~1 + MFCM).2
                                                   4.88066
                Dref(MOPLM, FOPLF, formula = ~1 + MFCM).3
                                                   4.83969
                Dref(MOPLM, FOPLF, formula = ~1 + MFCM).4
                                                   4.74849
                Dref(MOPLM, FOPLF, formula = ~1 + MFCM).5
                                                   4.42019
                Dref(MOPLM, FOPLF, formula = ~1 + MFCM).6
                                                   4.17956
                Dref(MOPLM, FOPLF, formula = ~1 + MFCM).7
                                                   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:

6.3 Uniform Difference (UNIDIFF) Models

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

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

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

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

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

```
> set.seed(1)
> data(yaish)
> unidiff <- gnm(Freq ~ educ * orig + educ * dest + Mult(Exp(-1 +
     educ), -1 + orig:dest), family = poisson, data = yaish, subset = (dest !=
     7))
Initialising
Running start-up iterations..
Running main iterations.....
Done
> coefs.of.interest <- grep("Mult1.Factor1", names(coef(unidiff)))</pre>
> coef(unidiff)[coefs.of.interest]
Mult1.Factor1.educ1 Mult1.Factor1.educ2 Mult1.Factor1.educ3 Mult1.Factor1.educ4
        -0.8242687
                            -1.0496405
                                              -1.5676923
                                                                  -1.8632073
Mult1.Factor1.educ5
        -3.0737713
```

The coefs.of.interest are 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:

```
Mult1.Factor1.educ3 -0.7434236 0.2335083 0.21182123 0.04486823
Mult1.Factor1.educ4 -1.0389386 0.3434256 0.32609379 0.10633716
Mult1.Factor1.educ5 -2.2495026 0.9453763 0.93560641 0.87535936
```

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 + Mult(Exp(-1 + election), religion:vote) + Mult(Exp(-1 +
      election), class:vote), family = poisson, data = cautres)
Initialising
Running start-up iterations..
Running main iterations.....
Done
> getContrasts(doubleUnidiff, rev(grep("Mult1.Factor1", names(coef(doubleUnidiff)))))
[[1]]
                                           SE
                          estimate
                                                 quasiSE
                                                            quasiVar
Mult1.Factor1.election4 0.00000000 0.00000000 0.07168290 0.005138439
Mult1.Factor1.election3 0.06682585 0.09906916 0.06812239 0.004640660
Mult1.Factor1.election2 0.24052778 0.09116479 0.05702819 0.003252214
Mult1.Factor1.election1 0.32834588 0.12213023 0.09803075 0.009610029
> getContrasts(doubleUnidiff, rev(grep("Mult2.Factor1", names(coef(doubleUnidiff)))))
[[1]]
                           estimate
                                           SE
                                                 quasiSE
                                                            quasiVar
Mult2.Factor1.election4
                         0.00000000 0.0000000 0.10934798 0.011956980
Mult2.Factor1.election3 0.08754435 0.1446833 0.09475938 0.008979340
Mult2.Factor1.election2 0.31990726 0.1320022 0.07395886 0.005469913
Mult2.Factor1.election1 -0.36183013 0.2534754 0.22854400 0.052232362
```

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 μ_{rc} a GAMMI-K model has the form

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

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

The row-column association models discussed in Section 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 5.4) 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)</pre>
> bilinear1 <- update(mainEffects, . ~ . + Mult(year - 1, treatment -</pre>
      1), start = c(coef(mainEffects), svdStart[, 1]))
Running main iterations
Done
We can compare the AMMI-1 model to the main effects model,
> anova(mainEffects, bilinear1)
Analysis of Deviance Table
Model 1: yield.scaled ~ year + treatment
Model 2: yield.scaled ~ year + treatment + Mult(year - 1, treatment -
  Resid. Df Resid. Dev
                        Df Deviance
1
        207
                279515
2
        176
                128383 31
                              151133
```

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 + Mult(site, variety, multiplicity = 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:

[1,] 4.1948212 -0.39186806 [2,] 2.7642419 -0.33951298 [3,] 1.4250456 -0.04654256 [4,] 1.8463067 0.33365981 [5,] 1.2704091 0.15776743 [6,] 1.1562916 0.40048225 [7,] 1.0172048 0.72727990 [8,] 0.6451366 1.46162702

[9,] -0.1470898 2.13234195

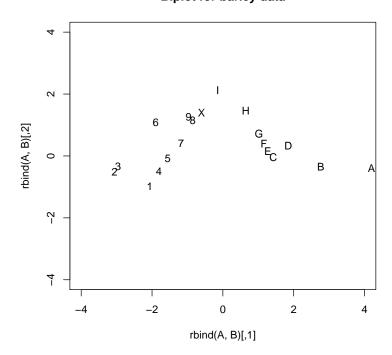
> B

```
[,1] [,2]
[1,] -2.0673655 -0.97420449
[2,] -3.0599788 -0.50683009
[3,] -2.9598021 -0.33190618
[4,] -1.8086251 -0.49758487
[5,] -1.5579480 -0.08444513
[6,] -1.8939998 1.08460534
[7,] -1.1790432 0.40687015
[8,] -0.8490092 1.14671353
[9,] -0.9704664 1.26558193
[10,] -0.6036790 1.39655898
```

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 \leftarrow pi/5

> rotation \leftarrow matrix(c(cos(a), sin(a), -sin(a), cos(a)), 2, 2,

+ byrow = TRUE)

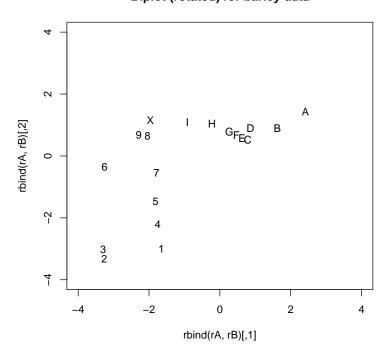
> rA \leftarrow (2 * A/3) \%\% rotation

> rB \leftarrow (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

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

$$\beta_j^T = \sqrt{(d)}(v_{1j}, v_{2j})$$

The rotated and scaled biplot suggests the simpler model

$$\alpha_i^T = (\gamma_i, 1)$$

$$\beta_i^T = (\delta_i, \tau_i)$$

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:

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

Initialising

Running start-up iterations..

Running main iterations.....

Done

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

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

[1] 9.513782 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
                         same
     1
        1 marked.improvement
> backPainLong <- expandCategorical(backPain, "pain")</pre>
> backPainLong[1:12, ]
    x1 x2 x3
                             pain count id
1
     1 1 1
                                        1
                            worse
                                      0
1.1
    1
       1 1
                             same
                                      1
                                        1
1.2
    1 1 1
               slight.improvement
                                        1
1.3 1 1 moderate.improvement
                                        1
1.4 1
              marked.improvement
       1
          1
                                        1
1.5
    1
       1
          1
                  complete.relief
                                         1
       1
                            worse
2.1 1
                             same
2.2 1 1
                                        2
          1
               slight.improvement
2.3 1
       1
          1 moderate.improvement
                                        2
2.4 1
              marked.improvement
                                        2
2.5
                  complete.relief
                                         2
```

We can now fit the stereotype model to these data:

Coefficients of interest:

```
painsame
                                                         painslight.improvement
                               16.1578
                                                                        15.6848
              painmoderate.improvement
                                                         painmarked.improvement
                               12.4555
                                                                        19.9140
                   paincomplete.relief
                                                        Mult1.Factor1.painworse
                               21.6653
                                                                        -0.2675
                Mult1.Factor1.painsame
                                          Mult1.Factor1.painslight.improvement
                                1.6657
                                                                         1.5614
Mult1.Factor1.painmoderate.improvement
                                          Mult1.Factor1.painmarked.improvement
                                1.1045
                                                                         2.1356
                                                               Mult1.Factor2.x1
     Mult1.Factor1.paincomplete.relief
                                2.5318
                                                                        -1.9190
                      Mult1.Factor2.x2
                                                               Mult1.Factor2.x3
                               -1.1007
                                                                        -0.9691
Deviance:
                     303.1003
Pearson chi-squared: 433.3727
Residual df:
using eliminate to handle the id factor so that these structural parameters do not appear in the model summaries. This
model is one dimensional since it involves only one function of \mathbf{x} = (x1, x2, x3). We can compare this model to one with
category-specific coefficients of the x variables, as may be used for a qualitative categorical response:
> threeDimensional <- gnm(count ~ pain + pain:(x1 + x2 + x3), eliminate = id,</pre>
      family = "poisson", data = backPainLong)
Initialising
Running main iterations.....
Done
> threeDimensional
Call:
gnm(formula = count \sim pain + pain:(x1 + x2 + x3), eliminate = id,
    family = "poisson", data = backPainLong)
Coefficients of interest:
                   painsame
                                  painslight.improvement
                    31.3062
                                                  30.9255
                                  painmarked.improvement
   painmoderate.improvement
                    27.8080
                                                  35.0086
        paincomplete.relief
                                             painworse:x1
                    37.4566
                                                   8.2129
                painsame:x1
                               painslight.improvement:x1
                    -2.9470
                                                  -2.6174
painmoderate.improvement:x1
                               painmarked.improvement:x1
                                                  -4.1771
     paincomplete.relief:x1
                                            painworse:x2
                    -4.6890
                                                   0.2552
                               painslight.improvement:x2
                painsame:x2
                    -2.4188
                                                  -2.2961
painmoderate.improvement:x2
                               painmarked.improvement:x2
                    -1.4168
                                                  -2.5886
```

painworse:x3

-1.9924

paincomplete.relief:x2

-3.0197

```
painsame:x3 painslight.improvement:x3
-3.1478 -3.2844
painmoderate.improvement:x3 painmarked.improvement:x3
-2.7386 -3.6838
paincomplete.relief:x3
-4.9330

Deviance: 299.0153
Pearson chi-squared: 443.0034
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
                           12
                                   -151.5501
threeDimensional
                           20
                                   -149.5076
```

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 ~ pain + Mult(pain - 1, x1 + x2 + x3 - 1),
    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	Pr(> z)
painsame	16.1578	6.5741	2.458	0.013980
painslight.improvement	15.6848	6.5274	2.403	0.016265
painmoderate.improvement	12.4555	6.4312	1.937	0.052777
painmarked.improvement	19.9140	6.4975	3.065	0.002178
paincomplete.relief	21.6653	6.5571	3.304	0.000953
Mult1.Factor1.painworse	-0.2675	NA	NA	NA
Mult1.Factor1.painsame	1.6657	NA	NA	NA
Mult1.Factor1.painslight.improvement	1.5614	NA	NA	NA
Mult1.Factor1.painmoderate.improvement	1.1045	NA	NA	NA

Mult1.Factor1.painmarked.improvement	2.1356	NA	NA	NA
Mult1.Factor1.paincomplete.relief	2.5318	NA	NA	NA
Mult1.Factor2.x1	-1.9190	NA	NA	NA
Mult1.Factor2.x2	-1.1007	NA	NA	NA
Mult1.Factor2.x3	-0.9691	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: 303.1 on 493 degrees of freedom

AIC: 731.1

Number of iterations: 15

Initialising

Running start-up iterations..

Running main iterations.....

Done

> summary(oneDimensional)

Call:

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	Pr(> z)
painsame	16.1578	6.5742	2.458	0.013980
painslight.improvement	15.6848	6.5274	2.403	0.016265
painmoderate.improvement	12.4556	6.4312	1.937	0.052777
painmarked.improvement	19.9140	6.4976	3.065	0.002178
paincomplete.relief	21.6653	6.5571	3.304	0.000953
Mult1.Factor1.painworse	1.3644	NA	NA	NA
Mult1.Factor1.painsame	-2.3453	NA	NA	NA
Mult1.Factor1.painslight.improvement	-2.1453	NA	NA	NA
Mult1.Factor1.painmoderate.improvement	-1.2685	NA	NA	NA
Mult1.Factor1.painmarked.improvement	-3.2472	NA	NA	NA
Mult1.Factor1.paincomplete.relief	-4.0074	NA	NA	NA
Mult1.Factor2.x2	0.5736	0.2178	2.633	0.008451
Mult1.Factor2.x3	0.5050	0.2431	2.077	0.037807

(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: 15

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, 6:11)

id6  id7  id8  id9  id10  id11
  NA  TRUE FALSE FALSE FALSE
Note: not all of the specified contrasts in this set are estimable
[[1]]
     Estimate Std. Error
id6      0  0.000000
id7      0  1.414214
```

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 $\alpha = 0$, $\beta = 0$, $\gamma = -0.1$.

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

Min. 1st Qu. Median Mean 3rd Qu. Max.
7.795e-16 8.099e-16 9.753e-16 1.590e+00 3.613e+00 3.613e+00
```

The saved.fits object thus contains the results of 100 calls to gnm, each using a different, randomly-generated starting value for the vector of parameters (α, β, γ) . The median deviance (in this case, residual sum of squares) among the 100 fits is essentially zero: in fact, 56 of these 100 fits reproduce the data exactly, to machine accuracy. The remaining 44 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 very first of the 100 fits is of this kind:

```
> saved.fits[[1]]
```

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):

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

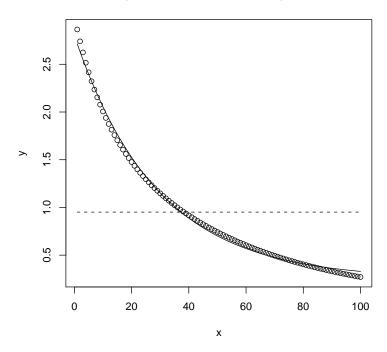
[1] 1.589496e-01 3.407062e-16 3.953716e-15 2.634119e-15 1.589496e-01
[6] 4.164390e+01 4.093554e-13 4.285232e-16 3.155106e-15 8.427057e-15
[11] 8.471544e-15 1.589496e-01 1.589496e-01
```

In this instance, only 13 of the 100 calls to gnm have successfully located a local maximum of the likelihood: in the remaining 87 cases the starting values generated were such that numerical problems resulted, and the fitting algorithm was abandoned (giving a NULL result). Among the 13 '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 8 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:

Deviance: 0.1589496
Pearson chi-squared: 0.1589496

Residual df: 97

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 γ_1 and γ_2 should both be small and negative, we might perhaps have tried

Coefficients:

Deviance: 6.690625e-15 Pearson chi-squared: 6.690625e-15

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 Fun	ctions
summary.gnm	summarize <i>gnm</i> fits
getContrasts	estimate contrasts and their standard errors for parameters in a gnm model
checkEstimable	check whether one or more parameter combinations in a gnm model is identified
exitInfo	print numerical details of last iteration when gnm has not converged
residSVD	multiplicative approximation of model residuals
se	get standard errors of linear parameter combinations in gnm 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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