# Generalized Nonlinear Models using the gnm Package

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#### Preface

Generalized linear models (logit/probit regression, log-linear models, etc.) are now part of the standard empirical toolkit.

Sometimes the assumption of a *linear* predictor is unduly restrictive.

This short course shows how *generalized nonlinear models* may be viewed as a unified class, and how to work with such models in R.

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Structured interactions

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RC Model with Heterogeneous Scores

Further Multiplicative Models

Diagonal Reference Model

Custom Nonlinear Terms

Practical II

# Part I

# Overview of Generalized Nonlinear Models in R

#### Linear models:

e.g.,

$$E(y_i) = \beta_0 + \beta_1 x_i + \beta_2 z_i$$

$$E(y_i) = \beta_0 + \beta_1 x_i + \beta_2 x_i^2$$

$$E(y_i) = \beta_0 + \gamma_1 \delta_1 x_i + \exp(\theta_2) z_i$$

In general:

$$E(y_i) = \eta_i(\beta) = \text{linear function of unknown parameters}$$

Also assumes variance essentially constant:

$$var(y_i) = \phi a_i$$

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with  $a_i$  known (often  $a_i \equiv 1$ ).

Background theory

#### Generalized linear models

Problems with linear models in many applications:

- range of y is restricted (e.g., y is a count, or is binary, or is a duration)
- effects are not additive
- ightharpoonup variance depends on mean (e.g., large mean  $\Rightarrow$  large variance)

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Background theory

Generalized linear model:

$$g[E(y_i)] = \eta_i = ext{linear function of unknown parameters} \ ext{var}(y_i) = \phi a_i V(\mu_i)$$

with the functions g (link function) and V (variance function) known.

# Background theory

#### Examples:

- binary logistic regressions
- rate models for event counts
- log-linear models for contingency tables (including multinomial logit models)
- multiplicative models for durations and other positive measurements
- hazard models for event history data

etc., etc.

#### e.g., binary logistic regression:

$$y_i = \begin{cases} 1 & \text{event happens} \\ 0 & \text{otherwise} \end{cases}$$

$$\mu_i = E(y_i) = \text{probability that event happens}$$

$$var(y_i) = \mu_i(1 - \mu_i)$$

Variance is completely determined by mean.

Common link functions are logit, probit, and (complementary) log-log, all of which transform constrained  $\mu$  into unconstrained  $\eta$ .

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e.g., multiplicative (i.e., log-linear) rate model for event counts.

'Exposure' for observation i is a fixed, known quantity  $t_i$ .

Rate model:

$$E(y_i) = t_i \exp(\beta_0) \exp(\beta_1 x_i) \exp(\beta_2 z_i)$$

i.e.

$$\log E(y_i) = \log t_i + \beta_0 + \beta_1 x_i + \beta_2 z_i$$

— effects are rate multipliers.

Variance is typically taken as the Poisson-like function  $V(\mu)=\mu$  (variance is equal to, or is proportional to, the mean).

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Generalized linear:  $\eta = g(\mu)$  is a linear function of the unknown parameters. Variance depends on mean through  $V(\mu)$ .

Generalized *nonlinear*: still have g and V, but now relax the linearity assumption.

Many important aspects remain unchanged

- ▶ fitting by maximum likelihood or quasi-likelihood
- ▶ analysis of deviance to assess significance of effects
- diagnostics based on residuals, etc.

But technically more difficult [essentially because  $\partial \eta/\partial \beta = X$  becomes  $\partial \eta/\partial \beta = X(\beta)$ ].

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#### Some practical consequences of the technical difficulties:

- ▶ automatic detection and elimination of redundant parameters is very difficult — it's no longer just a matter of linear algebra
- automatic generation of good starting values for ML fitting algorithms is hard
- great care is needed in cases where the likelihood has more than one maximum (which cannot happen in the linear case).

#### Some motivation: structured interactions

GNMs are not exclusively about structured interactions, but many applications are of this kind.

A classic example is log-linear models for structurally-square contingency tables (e.g., pair studies, before-after studies, etc.).

Pairs are classified twice, into row and column of a table of counts.

The independence model is

$$\log E(y_{rc}) = \theta + \beta_r + \gamma_c$$

or with glm

```
glm(y ~ row + col, family = poisson)
```

# Some standard (generalized linear) models for departure from independence are

quasi-independence,

```
y ~ row + col + Diag(row, col)
```

quasi-symmetry,

```
y ~ row + col + Symm(row, col)
```

symmetry,

```
y ~ Symm(row, col)
```

Functions Diag and Symm are provided by the **gnm** package along with the function Topo for fully-specified *topological* association structures, see ?Topo.

#### Row-column association

The uniform association model (for ordered categories) has

$$\log E(y_{rc}) = \beta_r + \gamma_c + \delta u_r v_c$$

with the  $u_r$  and  $v_c$  defined as fixed, equally-spaced scores for the rows and columns.

A natural generalization is to allow the *data* to determine the scores (Goodman, 1979). This can be done either heterogeneously,

$$\log E(y_{rc}) = \beta_r + \gamma_c + \phi_r \psi_c$$

or (in the case of a structurally square table) homogeneously

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# Introduction to the **gnm** package

The **gnm** package aims to provide a unified computing framework for specifying, fitting and criticizing generalized nonlinear models in R.

The central function is gnm, which is designed with the same interface as glm.

Since generalized linear models are included as a special case, the gnm function can be used in place of glm, and will give equivalent results.

For the special case  $g(\mu) = \mu$  and  $V(\mu) = 1$ , the gnm fit is equivalent to an nls fit.

#### Nonlinear model terms

Nonlinear model terms are specified in model formulae using functions of class "nonlin".

These functions specify the term structure, possibly also labels and starting values.

There are a number of "nonlin" functions provided by gnm. Some of these specify basic mathematical functions of predictors, e.g. Mult and Exp.

So heterogeneous row and column scores

$$\phi_r \psi_c$$

are specified as Mult(row, col).

#### There are two specialized "nonlin" functions provided by gnm

MultHomog: for homogeneous row and column scores, as in

$$\phi_r\phi_c$$

specified as MultHomog(row, col)

 ${ t Dref:}$  ' ${ t diagonal}$   ${ t reference'}$   ${ t dependence}$  on a  ${ t square}$   ${ t classification},$ 

$$w_1\gamma_r + w_2\gamma_c$$

(Sobel, 1981, 1985) specified as Dref(row, col)

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# Over-parameterization

The gnm function makes no attempt to remove redundant parameters from nonlinear terms. This is deliberate.

As a consequence, fitted models are typically represented in a way that is *over-parameterized*: not all of the parameters are 'estimable' (i.e., 'identifiable', 'interpretable').

For example, for the RC model with homogeneous scores

$$\alpha_r + \beta_c + \phi_r \phi_c = -k^2 + (\alpha_r - k\phi_r) + (\beta_c - k\phi_c) + (\phi_r + k)(\phi_c + k)$$
  
=  $\alpha_r^* + \beta_c^* + \phi_r^* \phi_c^*$ 

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gnm will return one of the infinitely many parameterizations at random.

#### Practical I

- 1. Load the **gnm** package. This provides the occupationalStatus data set, which is a contingency table classified by the occupational status of fathers (origin) and their sons (destination).
- 2. Use the generic function plot to create a mosaic plot of the table. Print occupationalStatus to see the cell frequencies represented by the plot.
- 3. If a table is passed to the data argument of gnm, it will be converted to a data frame with a column for each of the row and column factors and a column for the frequencies named Freq.

Use gnm to fit an independence model to these data (see p14), assigning the result to a suitable name. Print this object.

- 4. Type ?plot.gnm to open the help page on the gnm method for the plot function. Find out how to use plot to create a plot of residuals vs. fitted values and do this for the independence model. The poor fit should be very apparent!
- 5. Load the **vcdExtra** package. This provides the generic function mosaic, which has a method for "gnm" objects. Use this to visualize the goodness-of-fit of the independence model across the contingency table.
- 6. Fit a row-column association model with a homogeneous multiplicative interaction between origin and destination (see p16, p19). Check the fit with mosaic. Investigate the effect of modelling the diagonal elements separately, by adding Diag(origin, destination).

- 7. Keeping the Diag term in the model, use coef to access the coefficients and assign the result. Re-run the model fit and assign the coefficients of the re-fitted model to another name. Compare the coefficients side-by-side using cbind. Which parameters have been automatically constrained to zero? Which coefficients are the same in both models?
- 8. Standard errors can only be obtained for estimable parameters. Use summary to confirm which parameters are estimable in the current model. The homogeneous scores can be identified by setting one of them to zero. Re-fit the model using the argument constrain = "MultHomog(origin, destination)1". Compare the summary of the constrained model to the summary of the unconstrained model.

#### Part II

# Further Examples of Generalized Nonlinear Models

#### RC Model with Heterogeneous Scores

In this case, for example,

$$\alpha_r + \beta_c + \phi_r \psi_c = \alpha_r + (\beta_r - \psi_c) + (\phi_r + 1)\psi_c$$
$$= \alpha_r + \beta_c + (2\phi_r)(\psi_c/2)$$

so we need to constrain both the location and scale.

A standard convention is to constrain the scores so that

$$\sum_r \phi_r \pi_r = \sum_c \psi_c \pi_c = 0$$
 and 
$$\sum_r \phi_r^2 \pi_r = \sum_c \psi_c^2 \pi_c = 1$$

where  $\pi_r$  and  $\pi_c$  are the row and column probabilities respectively. The full interaction is then given by  $\sigma\phi_r\psi_c$ , where  $\sigma>0$  is the *intrinsic* association parameter.

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#### Example: Mental Health Data

1660 residents of Manhattan cross-classified by child's mental impairment and parents' socioeconomic status (Agresti, 2013).

```
xtabs(count ~ SES + MHS, mentalHealth)
     MHS
##
  SES well mild moderate impaired
        64
                      58
                               46
##
             94
##
        57 94
                      54
                               40
##
      57
            105
                      65
                               60
##
        72 141
                77
                              94
        36 97
                      54
                               78
##
        21
                               71
##
             71
                      54
```

We require treatment contrasts for the RC(1) mode

```
mentalHealth$MHS <- C(mentalHealth$MHS, treatment)
mentalHealth$SES <- C(mentalHealth$SES, treatment)</pre>
```

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    C 57 105
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                         78
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                  54
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```

We fit the RC(1) using the ofInterest argument to specify that only the parameters of the multiplicative interaction should be shown in model summaries.

```
RC <- gnm(count ~ SES + MHS + Mult(SES, MHS), family = poisson,
          data = mentalHealth, verbose = FALSE, ofInterest = "Mult")
coef (RC)
   Coefficients of interest:
          Mult(., MHS).SESA
                                    Mult(., MHS).SESB
##
##
                    0.77389
                                               0.78012
          Mult(., MHS).SESC
                                    Mult(., MHS).SESD
##
                    0.26620
                                              -0.00646
##
##
          Mult(., MHS).SESE
                                    Mult(., MHS).SESF
                   -0.67995
                                              -1.23326
##
##
       Mult(SES, .).MHSwell
                                 Mult(SES, .).MHSmild
##
                    0.41623
                                               0.04258
   Mult(SES, .).MHSmoderate Mult(SES, .).MHSimpaired
##
                    -0.02485
                                              -0.33519
```

The constraints that the weighted sum of column scores should sum to zero and the weighted sum of squares should sum to one are met by the scaled contrasts

$$\frac{\psi_c - \sum_c \psi_c \pi_c}{\sqrt{\sum_c \pi_c (\psi_c - \sum_c \psi_c \pi_c)^2}}$$

These contrasts can be obtained with <code>getContrasts</code> as follows:

```
## Mult(SES, .).MHSwell 1.678 0.194
## Mult(SES, .).MHSmild 0.140 0.200
## Mult(SES, .).MHSmoderate -0.137 0.280
## Mult(SES, .).MHSimpaired -1.414 0.172
```

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#### The row scores are computed in a similar way

Then the intrinsic association parameter can be computed directly

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

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#### Other Association Models

The row-column association models introduced so far are special cases of the RC(M) model:

$$\log(\mu_{rc}) = \alpha_r + \beta_c + \sum_{k=1}^{K} \sigma_k \phi_{kr} \psi_{kc},$$

Further association models include

- Models with skew-symmetric terms
- RC(M)-L models and UNIDIFF models for three-way tables

The **logmult** package enhances **gnm** by providing functions to support analyses involving log-multiplicative models.

Several models with multiplicative terms have been proposed outside of the context of association modelling.

Prominent examples include

- the stereotype model (Anderson, 1984), for ordered categorical response
- certain Rasch models, for item responses
- ▶ the Lee-Carter model (Lee and Carter, 1992) for mortality data

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Diagonal Reference Terms

Diagonal reference terms model the effect of factors with common levels. For factors indexed by i(f), the term is defined as

$$\sum_{f} w_{f} \gamma_{i(f)}$$

where  $w_f$  is a weight for factor f and  $\gamma_I$  is the diagonal effect for level I.

Unlike the GNMs models considered so far, which structure interaction terms, this structures the main effects of the corresponding factors.

Dref constrains the weights to be non-negative and to sum to one by defining them as

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

### Example: Conformity to parental rules

Data from a study of the value that parents place on their children conforming to their rules van der Slik *et al.* (2002).

Covariates are education level of mother and of father (MOPLM, FOPLF) plus 5 others.

Basic diagonal reference model for mother's conformity score (MCFM):

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

```
Diagonal Reference Model
```

```
A <- gnm(MCFM ~ -1 +

AGEM + MRMM + FRMF + MWORK + MFCM + Dref(MOPLM, FOPLF),

family = gaussian, data = conformity, verbose = FALSE)
```

In order for the diagonal weights to be identified, one of the  $\delta_f$  must be constrained to zero. DrefWeights computes the weights  $w_f$ , re-fitting the model constraining  $\delta_1 = 0$  if necessary:

```
w <- DrefWeights(A)
w

## $MOPLM
## weight se
## 0.423 0.144
##
## $FOPLF
## weight se
## 0.577 0.144</pre>
```

## Inference on the Weights

If the diagonal weights are near to 0.5, then a Normal approximation can be use to obtain a confidence interval, e.g.

```
w$MOPLM["weight"] + qnorm(c(0.025, 0.975)) * w$MOPLM["se"]
## [1] 0.140 0.705
```

Since  $0 < w_f < 1$ , a t-test is not a valid test of  $H_0$ :  $w_1 = 0$ . Instead use anova to compare against the implied GLM, e.g.

```
## Analysis of Deviance Table

##

## Model 1: MCFM ~ AGEM + MRMM + FRMF + MWORK + MFCM + FOPLF - 1

## Model 2: MCFM ~ AGEM + MRMM + FRMF + MWORK + MFCM + Dref(MOPLM, FOPLF)

## Resid. Df Resid. Dev Df Deviance Pr(>Chi)

## 1 577 428

## 2 576 425 1 2.9 0.048
```

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If the diagonal weights are near to 0.5, then a Normal approximation can be use to obtain a confidence interval, e.g.

```
w$MOPLM["weight"] + qnorm(c(0.025, 0.975)) * w$MOPLM["se"]
## [1] 0.140 0.705
```

Since  $0 < w_f < 1$ , a t-test is not a valid test of  $H_0$ :  $w_1 = 0$ . Instead use anova to compare against the implied GLM, e.g.

```
## Analysis of Deviance Table

##

## Model 1: MCFM ~ AGEM + MRMM + FRMF + MWORK + MFCM + FOPLF - 1

## Model 2: MCFM ~ AGEM + MRMM + FRMF + MWORK + MFCM + Dref(MOPLM, FOPLF)

## 1

## Resid. Df Resid. Dev Df Deviance Pr(>Chi)

## 1 577 428

## 2 576 425 1 2.9 0.048
```

The Dref function allows dependence of the weights on other variables. van der Slik *et al.* (2002) consider weights dependent upon mother's conflict score (MFCM), as in

$$\delta_k = \xi_k + \phi_k x_5 \qquad (k = 1, 2)$$

which can be specified in R as

```
F <- gnm(MCFM ~ -1 + AGEM + MRMM + FRMF + MWORK + MFCM +

Dref(MOPLM, FOPLF, delta = ~ 1 + MFCM),

family = gaussian, data = conformity, verbose = FALSE)
```

Diagonal Reference Model

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).

```
## $MOPLM
## MFCM weight se
## 1  1 0.0297 0.228
## 2  0 0.7447 0.201
##
## $FOPLF
## MFCM weight se
## 1  1 0.970 0.228
## 2  0 0.255 0.201
```

#### Custom "nonlin" Functions

A ""nonlin"" function creates a list of arguments for the internal function nonlinTerms.

The term is viewed as a function of

predictors linear predictors with coefficients to be estimated, including the special case of single parameters

variables variables included in the term with a coefficient of 1

### Example: Modelling Prey Consumption

A ecology student wished to use the Holling Type II function to model the number of prey eaten by a certain predator in a given time period:

$$y(x) = \frac{ax}{1 + ahx}$$

where x is the number of prey at the start of the experiment, a is the attack rate and h is the time the predator spends handling the prey.

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The model can be broken down into predictors and variables as follows

$$\frac{ax}{1+\{a\}\{h\}x}$$

We start to build our nonlin function as follows:

```
TypeII <- function(x){
  list(predictors = list(a = 1, h = 1),
      variables = list(substitute(x)))
}
class(TypeII) <- "nonlin"</pre>
```

The term argument of nonlinTerms takes labels for the predictors and variables and returns a departed expression of the term:

#### Or using sprintf

#### Complete Function

Some test data were provided:

```
Density <- rep(c(2,5,10,15,20,30), each = 4)
Eaten <- c(1,1,0,0,2,2,1,1,1,2,3,2,2,2,3,3,3,3,4,3,3,3,4,3)
```

The counts are expected to be underdispersed so we use the quasipoisson family with link = "identity". Both a and h should be positive, so we provide starting values

```
Custom Nonlinear Terms
```

##

```
## Call:
##
## gnm(formula = Eaten ~ -1 + TypeII(Density), family = quasipoisson(link
      start = c(a = 0.1, h = 0.1))
##
##
## Deviance Residuals:
      Min 1Q Median 3Q Max
##
## -1.1154 -0.2854 -0.0166 0.3345 0.5938
##
## Coefficients:
    Estimate Std. Error t value Pr(>|t|)
##
## a 0.3546 0.0778 4.56 0.00016
## h 0.1975 0.0415 4.76 9.5e-05
##
  (Dispersion parameter for quasipoisson family taken to be 0.208)
##
## Residual deviance: 5.7279 on 22 degrees of freedom
## AIC: NA
##
## Number of iterations: 7
```

### Incorporating dependence

The parameters a and h can be allowed to depend on a factor as follows

```
Catchment <- factor(rep(1:2, 6, each = 2))
mod2 <- gnm(Eaten ~ -1 + TypeII(Catchment, Density),</pre>
            start = rep(0.2, 4),
            family = quasipoisson(link = "identity"))
## Running main iterations......
## Done
coef (mod2)
## Coefficients:
## aCatchment1 aCatchment2 hCatchment1 hCatchment2
        0.697
                    0.246
                                 0.318
                                             0.107
##
```

If instead we wanted to allow a general predictor to be supplied by the user as a formula we would use

Note additional parentheses!

```
mod2 <- gnm(Eaten ~ -1 + TypeII(~ 1 + Catchment, Density),</pre>
           start = c(0.2, -0.1, 0.2, -0.1),
           family = quasipoisson(link = "identity"))
  Running main iterations.....
## Done
coef (mod2)
  Coefficients:
  a(Intercept) aCatchment2 h(Intercept) hCatchment2
         0.697 -0.451
                                  0.318
                                             -0.211
##
```

#### Practical IIa

1. The voting data in gnm are from the 1987 British general election. The data frame comprises the percentage voting Labour (percentage), the total number of people (total), the class of the head of household (destination) and the class of their father (origin). We shall fit a diagonal reference model to these data.

First we want to convert percentage into a binomial response. So that gnm will automatically weight the proportion of successes by the group size, we choose to do this by creating a two-column matrix with the columns giving the number of households voting Labour ('success') and the number of households voting otherwise ('failure'):

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

- 2. Use gnm to model yvar by a diagonal reference term based on origin and destination (see p35), with family = binomial. Look at the summary does the model fit well? Use the mosaic function from vcdExtra to examine the residuals over the origin by destination table. Since the data were not provided to gnm as a table, you will need to provide a formula with the cross-classifying factors.
- 3. It could be that the diagonal weights should be different for the upwardly mobile. Define a variable to indicate this group as follows:

```
origin <- as.numeric(as.character(voting$origin))
destination <- as.numeric(as.character(voting$destination))
upward <- origin > destination
```

Using this variable, refit the diagonal reference model to have separate weights for the upwardly and downwardly mobile (note the stable are modelled by the diagonal effects). Do the weights differ between the two groups?

4. It could be that individuals which have come into or out of the salariat (class 1) vote differently from other individuals. Define variables indicating movement in and out of class 1 as follows:

```
in1 <- origin != 1 & destination == 1
out1 <- origin == 1 & destination != 1</pre>
```

Re-fit the diagonal reference model, specifying  $\sim 1 + \text{in}1 + \text{out}1$  as the formula argument of Dref, so the weights are parameterized by a main effect with additional effects for in1 and out1.

5. Evaluate the weights under the new model. The weights for groups that have moved in to the salariat are similar to the general weights. Fit a model that only has separate weights for the groups moving out of the salariat. Is this model a significant improvement on the standard diagonal reference model?

#### Practical IIb

1. The generalized logistic function or Richard's curve is defined as

$$y(t) = A + \frac{K - A}{(1 + \exp(-B(t - M))^{1/\nu})}$$

where

A is the lower asymptote

K is the upper asymptote

B is the growth rate

v affects near which asymptote the growth rate is at its maximum

M is the time at which the growth rate is at its maximum

Create a custom ""nonlin"" function to fit this model.

Some test data are provided in the file Richard.txt in the data folder of the course materials. Plot y against t. Since y decreases as t increases (i.e. the growth rate is negative) the upper asymptote is the value as  $t \to -\infty$  and the lower asymptote is the value as  $t \to \infty$ . Given that if v = 1, M is the value of t at which y is half-way between the lower and upper asymptotes, make reasonable guesses for starting values of A, K, B, v and M. Use gnm to fit the Richard's curve to these data, with family = gaussian and start set to your guessed values. Note the starting values must be in the same order as specified by the predictors element of your "nonlin" term.

Practical II

3. Add the fitted line to your plot. Does the model fit well? Look at the summary for your fitted model. Are all the parameters significant? Investigate whether one or more of the following simplifications is reasonable:

- $\triangleright$  v=1
- ightharpoonup A = 0
- K = 100

### Concluding Remarks

Many frequently-used GNMs can be handled by gnm and convenience functions for association models are available in **logmult**.

Other examples in the gnm vignette/documentation include

- GAMMI models (RC(M) models for a general response)
- biplot models for two-way data
- compound exponential decay curves
- double UNIDIFF model for 4-way table ?cautres

Formula interface to gnm encourages experimentation and uninhibited modelling.

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