Nonparametric maximum likelihood estimation for random effect models in R

Vignette to R package **npmlreg**

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1 Introduction

approach is that the random effect distribution does not need to be specified a priori, whereas the huge body of literature on GLMMs restricts nearly exclusively on normally distributed random effects. Further, complicated integrations are avoided by approximating the marginal likelihood by a simple finite mixture, for which standard fitting algorithms based on EM exist and can be applied. NPML for generalized linear models with random effects was previously implemented by Aitkin & Francis (1995) in the GLIM4 language, which is however no longer widely used. The main functions of this package, alldist (for overdispersion) and allve (for variance component Nonparametric maximum likelihood (NPML) estimation is an attractive tool for the fitting of generalized linear models with random effects, which can be considered as a special case of generalized linear mixed models (GLMMs). One crucial advantage of the NPML models), are modified and extended versions of their homonymous counterparts in GLIM4, and have been translated to R originally by In this handbook the concept of NPML estimation is briefly explained (Section 2) and a variety of data examples are given (Section 3), which illustrate the functionalities of alldist and allvc. The R package npmlreg is available for download on CRAN at

Key Words: Varying coefficient models, random effect models, mixed models, mixture models, Gaussian Quadrature, EM algorithm, Two-level models, exponential family regression models.

2 Random effect modelling with exponential family mixtures

Assume there is given a set of explanatory vectors x_1, \ldots, x_n and a set of observations y_1, \ldots, y_n sampled from an exponential family distribution $f(y_i|\beta,\phi_i)$ with dispersion parameter ϕ_i . In a generalized linear model, predictors and response are assumed to be related through a link function h,

$$\mu_i \equiv E(y_i|\beta,\phi_i) = h(\eta_i) \equiv h(x_i'\beta),$$

and the variance $Var(y_i|\beta,\phi_i)=\phi_iv(\mu_i)$ depends on a function $v(\mu_i)$ which is entirely determined by the choice of the particular exponential family. However, often the actual variance in the data is larger than the variance according to this strict mean-variance

¹In the present implementation of alldist, Gausssian, Poisson, Binomial, and Gamma distributed response are supported.

relationship. This effect is commonly called overdispersion. Reasons for overdispersion might be e.g. correlation in the data or important explanatory variables not included in the model. In order to account for additional unexplained variability of the individual observations, a random effect z_i with density g(z) is included into the linear predictor²

$$\eta_i = \beta' x_i + z_i.$$

The marginal likelihood can now be written as

$$L = \prod_{i=1}^{n} \int f(y_i|z_i, \beta, \phi_i) g(z_i) dz_i$$

$$\tag{1}$$

and can be approximated by a finite mixture
$$\prod_{i=1}^n \left\{ f(y_i|z_i,\beta,\phi_i)g(z_i) \, dz_i \right\}$$
 and can be approximated by a finite mixture
$$\prod_{i=1}^n \left\{ \sum_{k=1}^K f(y_i|z_k,\beta,\phi_k)\pi_k \right\} \equiv \prod_{i=1}^K \left\{ \sum_{k=1}^K f_{ik}\pi_k \right\},$$
 where z_k are the mass points and π_k their masses. The log-likelihood is then given by
$$\ell = \sum_{i=1}^n \log \left\{ \sum_{k=1}^K \pi_k f_{ik} \right\}.$$
 The score equations

$$\ell = \sum_{i=1}^n \log \left\{ \sum_{k=1}^K \pi_k f_{ik}
ight\}.$$

 $\overline{\mathfrak{S}}$

The score equations
$$\frac{\partial \ell}{\partial z_k} = 0, \quad \frac{\partial \ell}{\partial \beta} = 0,$$
 turn out to be weighted versions of the single-distribution score equations, with weights

(3)

$$w_{ik} = \frac{\pi_k f_{ik}}{\sum_{\ell} \pi_{\ell} f_{i\ell}}.$$
 (4)

²We refer to a model defined in this manner as a generalized linear model with random effect, or shorter, random effect model, whereas the more general linear predictor $\eta_i = \beta' x_i + \gamma'_i \tilde{x}_i$, with γ_i random and \tilde{x}_i typically being a subvector of x_i , entails a generalized linear mixed model.

The weights w_{ik} can be interpreted as posterior probabilities that the observation y_i comes from component k. The score equation for the mixture proportions,

$$\frac{\partial \ell - \lambda(\sum \pi_k - 1)}{\partial \pi_k} = 0,$$

gives the ML estimate

$$\hat{\pi_k} = rac{1}{n} \sum_i w_{ik}$$

 $\widehat{\mathbf{c}}$

which can be nicely interpreted as the average posterior probability for component k. The parameters ϕ_k , β , z_k and π_k can now be simultaneously estimated by an standard EM algorithm:

Starting points Select starting values $\phi^{(0)}$, $\beta^{(0)}$, $z_k^{(0)}$, and $\pi_k^{(0)}$, k = 1, ..., K.

E-Step Adjust weights using formula (4) with current parameter estimates.

M-Step Update parameter estimates fitting a weighted GLM with weights w_{ik} , including mass points as dummy variables.

corresponding masses for z_k and π_k , respectively, and consider these values as constants (Hinde, 1982). Otherwise, they have to be which are scaled outwards (tol >1) or inwards (tol <1) by means of a scaling parameter tol). As in this case no parametric specification (Laird, 1978), which was adapted to the framework of overdispersed generalized linear models by Aitkin (1996a). In difference to the original implementation in GLIM4, we use a 'damping' procedure in the initial cycles of the algorithm, which reduces the sensitivity of the In the special case of a normally distributed random effect, one can employ tabulated Gauss-Hermite integration points and their calculated simultaneously during the EM algorithm as outlined above (one then usually takes the GH points/masses as starting points, of the random effect distribution is necessary, one refers to this method as 'Nonparametric Maximum Likelihood' (NPML) estimation EM algorithm to the optimal choice of tol for exponential family densities possessing a dispersion parameter (as Gaussian or Gamma). For technical details on the implementation of the algorithm, see Einbeck & Hinde (2006)

Examples

3.1 Finite Gaussian mixtures: The galaxy data

galaxies. Note that, in this dataset, there is a typo in the 78th observation, which should be 26960 instead of 26690. We correct this to separated conic sections of space. The full data were given by Postman et al. (1986). They are part of the R package MASS as data set The data considered in this example are the recession velocities (in km/s) of 82 galaxies receding from our own, sampled from six wellobtain consistent and comparable results with those presented in Aitkin et al. (2005) and other references.

```
> data(galaxies, package = "MASS")
> galaxies[78] <- 26960
> gal <- as.data.frame(galaxies)</pre>
```

> rm(galaxies)

Next, we construct a new variable v1000 from galaxies, which represents the velocity in units of $10^3 km/s$:

```
21.960
22.888
                                                  [11] 18.552 18.600 18.927 19.052 19.070 19.330 19.343 19.349 19.440 19.473
                                                               19.663 19.846 19.856 19.863 19.914 19.918 19.973
                                     9.558 9.775 10.227 10.406 16.084 16.170 18.419
                                                                             20.795
                                                                             20.415 20.629
                                                                                          21.814 21.921
                                                                                                        22.746 22.747
                                                                                                                     23.706
                                                                             20.179 20.196 20.215 20.221
                                                                                                         22.495
                                                                                                                      23.542
                                                                                          21.492 : 22.374 :
                                                                                                                     23.538
                                                                                                                                   24.990
                                                                                          20.986 21.137
                                                                                                        22.314
                                                                                                                     23.484
                                                                                                                                   24.717
> gal$v1000 <- gal$galaxies/1000
                                     9.350 9.483
                                                                19.547
                                                                             20.175
                                                                                          20.875
                                                                                                        22.242
                                                                                                                     23.241
                                                                19.529 19.541
                                                                             20.166
                                                                                                       22.209
                                                                                                                     23.206
                                                                                          20.846
                                    9.172
                                                                             19.989
                                                                                                        22.185
                                                                                                                     22.914
                                                                                          20.821
                                                                                                                                   24.129
            > gal$v1000
                                     [1]
                                                                [21]
                                                                             [31]
                                                                                           [41]
                                                                                                        [51]
                                                                                                                     [61]
                                                                                                                                   [71]
```

and load the **npmlreg** package:

```
random.distribution = "np")
                                                                                                                                                                                                                                                                                                                                                                                                                                          which is the same as a NPML estimation with one mass point, fitting a 'mixture' of one normal component:
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  > (galaxy.np1 <- alldist(v1000 \degree 1, random = \degree1, random.distribution = "np",
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             Call: alldist(formula = v1000 ~ 1, random = ~1, data = gal, k = 1,
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                0
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              4.568
                                                                                                                                                                                                                                                                                                                 Degrees of Freedom: 81 Total (i.e. Null); 81 Residual
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            Random effect distribution - standard deviation:
                                                                                                                Call: glm(formula = v1000 ~ 1, data = gal)
                                                                                                                                                                                                                                                                                                                                                                                AIC: 484.8
Fitting a simple constant normal model yields
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              Component distribution - MLE of sigma:
                                                    > glm(v1000 ~ 1, data = gal)
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   k = 1, data = gal)
                                                                                                                                                                                                                                                                                                                                                                                Residual Deviance: 1690
                                                                                                                                                                                                                                                                                                                                                 Null Deviance:
                                                                                                                                                                                   Coefficients:
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               Coefficients:
                                                                                                                                                                                                                                                 20.83
                                                                                                                                                                                                                 (Intercept)
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           MASS1
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            20.83
```

> library(npmlreg)

Mixture proportions:

MASS1

-

-2 log L: 480.8

The option data=.... is mandatory, even if the data frame was attached to the workspace! The deviance can be obtained by

> galaxy.np1\$dev

[1] 1690.296

which is certainly the same as for the GLM. Next, we fit discrete mixtures $\sum_{k=1}^{K} \pi_k f_k$, where the f_k are normal densities with expectation μ_k and unknown, but equal variances $\sigma^2 = \sigma_k^2$. Fitting models with K = 2, 3, 4, and 5 mass points, one obtains

> (galaxy.np2 <- alldist(v1000 ~ 1, random = ~1, random.distribution = "np",

+ k = 2, data = gal)

1 ..2 ..3 ..4 ..5 ..6 ..7 ..8 ..9 ..10 ..11 ..12 ..13 ..14 ..15 ..16 ..17 ..18 ..19 ..20 ..21 ..22 ..23 ..24 ..25 ..26 ..27 ..28 ..29 ..30

EM algorithm met convergence criteria at iteration # 37

Disparity trend plotted.

EM Trajectories plotted.

random.distribution = "np") Call: alldist(formula = v1000 ~ 1, random = ~1, data = gal, k = 2,

Coefficients:

MASS1 MASS2

9.865 21.876

Component distribution - MLE of sigma: 3.026

Random effect distribution - standard deviation: 3.384072

```
random.distribution = "np")
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       > (galaxy.np4 <- alldist(v1000 ~ 1, random = ~1, random.distribution = "np", + k = 4. data = $\sigma1))
                                                                      > (galaxy.np3 <- alldist(v1000 ~ 1, random = ~1, random.distribution = "np",
                                                                                                                                                                                                                                                                                          Call: alldist(formula = v1000 ~ 1, random = ~1, data = gal, k = 3,
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           4.036180
                                                                                                                                                                            EM algorithm met convergence criteria at iteration # 10
                                                                                                                                                                                                                                                                                                                                                                                                                                                                2.079
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           Random effect distribution - standard deviation:
                                                                                                                                                1 ..2 ..3 ..4 ..5 ..6 ..7 ..8 ..9 ..10 ..
                                                                                                                                                                                                                                                                                                                                                                                                                                                              Component distribution - MLE of sigma:
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            MASS3
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        0.08590000 0.87690389 0.03719611
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          k = 4, data = gal)
                                                                                                  k = 3, data = gal)
                                                                                                                                                                                                         Disparity trend plotted.
                                                                                                                                                                                                                                     EM Trajectories plotted.
0.91305867
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    Mixture proportions:
                                                                                                                                                                                                                                                                                                                                                                                                        32.94
                                                                                                                                                                                                                                                                                                                                                                             MASS1 MASS2 MASS3
                                                                                                                                                                                                                                                                                                                                                   Coefficients:
                                                                                                                                                                                                                                                                                                                                                                                                       9.75 21.40
0.08694133
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              MASS1
                           -2 log L:
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   -2 log L:
```

Mixture proportions:

1 ..2 ..3 ..4 ..5 ..6 ..7 ..8 ..9 ..10 ..11 ..12 ..13 ..14 ..15 ..16 ..17 ..18 ..

EM algorithm met convergence criteria at iteration # 18

Disparity trend plotted.

EM Trajectories plotted.

random.distribution = "np") Call: alldist(formula = v1000 ~ 1, random = ~1, data = gal, k = 4,

Coefficients:

MASS1 MASS2 MASS3 MASS4

71 20.00 23.50 33.04

Component distribution - MLE of sigma: 1.315

Random effect distribution - standard deviation: 4.345212

Mixture proportions:

S1 MASS2 MASS3 MASS4

0.08536797 0.52624187 0.35180277 0.03658738

; log L: 416.

and observes a steady decrease in disparity, i.e. $-2\log L$. As a by-product, the alldist routine produces a plot showing how the disparity converges (Fig. 1 top), and another plot showing the EM trajectories (Fig. 1 bottom).

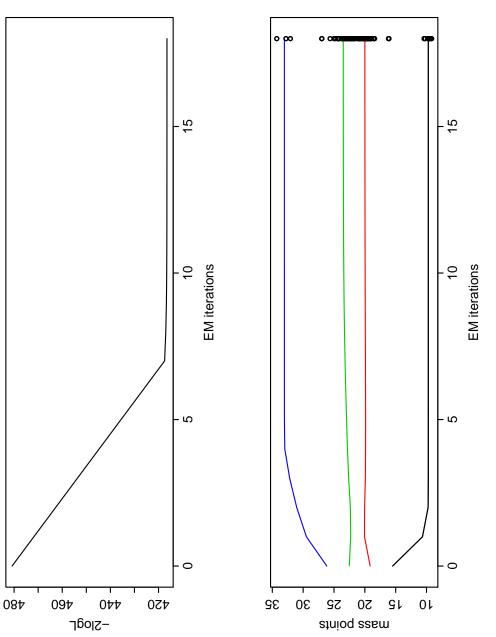


Fig. 1: Convergence of EM algorithm for NPML estimation with 4 mass points. Top: Disparities; Bottom: EM Trajectories.

As random.distribution='np' is the default setting, it can be omitted. For 5 to 9 mass points, we only report the disparity values

```
> (galaxy.np5 <- alldist(v1000 ~ 1, random = ~1, k = 5, data = gal, + verbose = FALSE))$disp
```

[1] 410.6852

```
> (galaxy.np6 <- alldist(v1000 \degree 1, random = \degree1, k = 6, tol = 0.2, + data = gal, verbose = FALSE))$disp
```

[1] 394.5811

```
> (galaxy.np7 <- alldist(v1000 ~ 1, random = ~1, k = 7, tol = 0.12,
```

data = gal, verbose = FALSE)

[1] 388.8639

```
> (galaxy.np8 <- alldist(v1000 ~ 1, random = ~1, k = 8, tol = 0.2,
```

data = gal, verbose = FALSE)

[1] 388.177

$$> (galaxy.np9 <- alldist(v1000 ~ 1, random = ~1, k = 9, tol = 0.06,$$

data = gal, verbose = FALSE))\$disp

[1] 388.2149

tol to obtain the disparity values given above. The tol parameter influences the position of the starting points, where values tol < 1mean concentrated values compared to the default setting (Gaussian quadrature points). The disparity values for 2 and 5 mass points are better than those obtained by Aitkin (2001) with GLIM 4. One reason for that is the applied damping procedure: As the algorithm is indicating that the disparity stabilizes at about 8 mass points. Note that in some cases it was necessary to modify the optional parameter

less sensitive to the optimal choice of tol, the optimal solutions are found more easily. An assisting tool in the selection of tol is the R function tolfind included in the package npmlreg.

To fit a Gaussian mixture with unequal standard deviations σ_k , $k=1,\ldots,K$ varying over the components, the possibility of smoothing the standard deviations among components is implemented. Smoothing is performed by means of the discrete kernel

$$W(x,y|\lambda) = \left\{ \begin{array}{ll} \lambda & \text{if} \quad y = x \\ (1-\lambda)/(K-1) & \text{if} \quad y \neq x \end{array} \right.$$

(Aitchison and Aitken, 1976). The setting $\lambda = 1/K$ corresponds to the extreme case 'maximal smoothing' (i.e. equal variances $\sigma^2 = \sigma_{k}^2$.), while $\lambda = 1$ means that all standard deviations are calculated within the components (i.e. unequal variances σ_k^2). Statistically sensible settings are only $1/K \le \lambda \le 1$. The default setting $\lambda = 0$ is automatically mapped to $\lambda = 1/K$.

As an example, we compute the four mass-points model with option lambda=1

```
> summary(galaxy.np4u <- alldist(v1000 \degree 1, random = \degree1, k = 4,
+ tol = 0.5, data = gal, lambda = 1, verbose = FALSE))
```

tol = 0.5, lambda = 1, verbose = FALSE) Call: alldist(formula = $v1000 \ ^{\circ}$ 1, random = $^{\circ}$ 1, data = gal, k = 4,

Coefficients:

Estimate Std. Error t value MASS1 9.710143 0.2776679 34.97035 MASS2 19.949549 0.1174379 169.87311 MASS3 23.135282 0.1281410 180.54545 MASS4 33.044336 0.4241453 77.90805

Mixture proportions:

MASS1 MASS2 MASS3 MASS4 0.08536585 0.47707433 0.40097456 0.03658525

MLE of component standard deviations:

MASS1 MASS2 MASS3 MASS4 0.4225107 1.3831150 1.6866727 0.9217176 Random effect distribution - standard deviation:

-2 log L: 405 Convergence at iteration 31

One gets deeper insight into the fitted model looking at diagnostic plots. Calling

> plot(galaxy.np4u, plot.opt = 15, height = 5)

gives the disparities and EM trajectories as above (Fig. 2 top), and additionally two plots showing the empirical Bayes predictions vs the true responses, and the component posterior probabilities (w_{ik}) against the fixed part residuals $(y_i - x_i \beta)$, respectively. In the former plot Fig. 2 left bottom), one sees nicely how the predicted values are 'flattened' within the custers and smoothed between. In the latter plot (Fig. 2 right bottom), one gets an impression of the discriminatory power of the mixture components. Throughout all plots, one colour corresponds to the same particular mass point.

in a somewhat makeshift manner using the equal dispersion parameter for the ϕ preceding the log-likelihood, and the unequal dispersion An important remark should be given here: Interpretation (and definition!) of the deviance $D = -2\phi \log L + 2\phi \log L$ solven provided in \$deviance, is not clear when using unequal dispersion parameters. In the present implementation, deviances are calculated in this case parameters within the log-likelihood. Hence, it is strictly recommended to work with the disparity rather with the deviance in the case of unequal component dispersion parameters, as the the disparity does not share this problem. This is also the reason why we prefer to work with disparities in general, and why disparities (and not deviances) are displayed in the summaries.

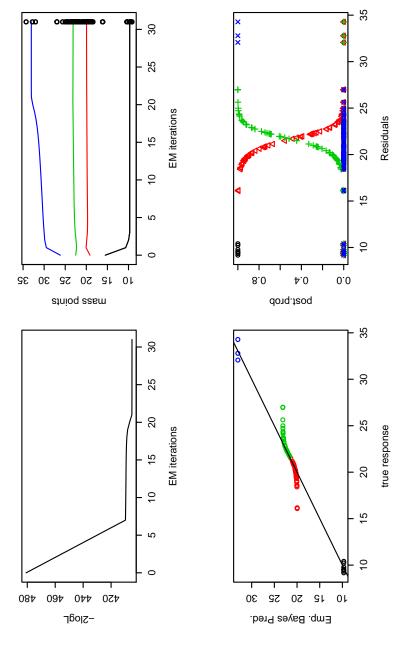


Fig. 2: Diagnostic plots for NPML estimation with unequal variances and 4 mass points.

One might fear that for a high number of mass points some component standard deviations could tend to zero. This can indeed be the case. Using 8 instead of 4 mass points in the call above one gets the error message

Check model specification, enable spike protection or smooth among components. Error in alldist(v1000 1, random = 1, k = 8, tol = 0.5, data = gal, Singularity or Likelihood-Spike at iteration #12.

disparity 357.8, which is a good part better then the value given in Aitkin (2001), 361.0. If likelihood spikes occur for any tol, one can This problem may be solved, as a first attempt, by modifying tol. In this case, tol=0.32 gives a likelihood-spike free solution with enable the spike protection (spike.protect=1), which stops the algorithm as soon as one component starts to enter a likelihood spike. For instance, running

tol = 0.5, lambda = 1, spike.protect = TRUE, verbose = FALSE) data = gal, lambda = 1, verbose = FALSE, spike.protect = TRUE)) > (galaxy.np8us <- alldist(v1000 $^{\circ}$ 1, random = $^{\circ}$ 1, k = 8, tol = 0.5, Call: alldist(formula = v1000 ~ 1, random = ~1, data = gal, k = 8,

MASS4 MASS3 MASS2 Coefficients: MASS1

906.6

9.383

MASS8 34.279 32.433 MASS7 24.410 MASS6 MASS5 22.587 19.772 17.233

4.417512 Random effect distribution - standard deviation:

Mixture proportions:

0.11323979 0.03637014 0.37478549 0.35365507 MASS5 MASS4 MASS3 0.05078828 MASS2 0.03457724

MASS8 MASS7

0.01219512 0.02438886

324.3 -2 log L:

> galaxy.np8us\$sdev\$sdevk

```
[1] 1.504988e-01 4.113445e-01 1.526060e+00 6.309877e-01 1.170915e+00
```

[6] 1.738375e+00 3.757823e-01 7.105427e-15

care, as the displayed disparity is normally not correct when the algorithm does not have converged. One notices from this output that gives us estimates of mass points, masses, and standard deviations of the mixture components. These values have to be interpreted with the 8th mass point is responsible for the likelihood spike.

The better approach is to set the smoothing parameter equal to $\lambda = 0.99$, which corresponds to unequal standard deviations with a very low amount of smoothing among components:

```
> (galaxy.np8ud <- alldist(v1000 \degree 1, random = \degree1, k = 8, tol = 0.5,
```

data = gal, lambda = 0.99))

1 ... 2 ... 3 ... 4 ... 5 ... 6 ... 7 ... 8 ... 9 ... 10 ... 11 ... 12 ... 13 ... 14 ... 15 ... 16 ... 17 ... 18 ... 19 ... 20 ... 21 ... 22 ... 23 ... 24 ... 25 ... 26 ... 27

..28 ..29 ..30

7 EM algorithm met convergence criteria at iteration # 102

Disparity trend plotted.

EM Trajectories plotted.

tol = 0.5, lambda = 0.99) ∞ Call: alldist(formula = v1000 ~ 1, random = ~1, data = gal, k =

Coefficients:

MASS1 MASS2 MASS3 MASS4 MASS5 MASS6 MASS7 MASS8

9.836 9.710 16.127 19.790 22.922 26.978 32.427 34.279

Random effect distribution - standard deviation: 4.448856

Mixture proportions:

MASS1 MASS2 MASS3 MASS4

7.888540e-15 8.536585e-02 2.439018e-02 4.039238e-01 4.256102e-01

MASS8 2.439092e-02 1.219444e-02 MASS7 2.412464e-02 MASS6 -2 log L:

> galaxy.np8ud\$sdev\$sdevk

[1] 0.9061662 0.4349857 0.2183475 0.6758124 1.2048199 0.2160915 0.4119882 [8] 0.2949645

The motivation for the implementation of spike. protect is mainly to enable to run tolfind without breaking down if likelihood spikes occur. Hence, it is in alldist by default switched off, and in tolfind by default switched on. The result of tolfind for the 8-mass point model with unequal variances is shown in Fig. 2: Red circles correspond to tol values where the spike protection had to interfere and hence the EM algorithm did not converge. Only disparity values associated with green circles are reliable, and the optimal value of tol should consequently be chosen from them.

```
find.in.range = c(0, 0.6), steps = 12, plot.opt = 0, verbose = FALSE,
                                                                                                                                                                                                                                 360.9393 359.4521 357.8221
                         > tolfind(v1000 ^{\circ} 1, random = ^{\circ}1, k = 8, data = gal, lambda = 1,
                                                                                                                                                                                                                                                                                                                                                   [1] 0.05 0.10 0.15 0.20 0.25 0.30 0.35 0.40 0.45 0.50 0.55 0.60
                                                                                                                                                                     Minimal Disparity with EM converged: 357.8216 at tol= 0.4
                                                                                                                                                                                                                                 377.0345
                                                                                                                                                                                                                                                        363.8772
                                                                                                                                       Minimal Disparity: 323.3126 at tol= 0.45
                                                                                                                                                                                                                                                            324.2868
                                                                                                                                                                                                                                 377.6917
> par(mfrow = c(1, 1), cex = 0.65)
                                                                                  noformat = TRUE)[c(3, 4)]
                                                                                                                                                                                                                             387.2360
                                                                                                                                                                                                                                                          323.3126
                                                                                                                                                                                                    $AllDisparities
                                                                                                                                                                                                                             [1] 1233.6883
[8] 357.8216
                                                                                                                                                                                                                                                                                                                      $Alltol
```

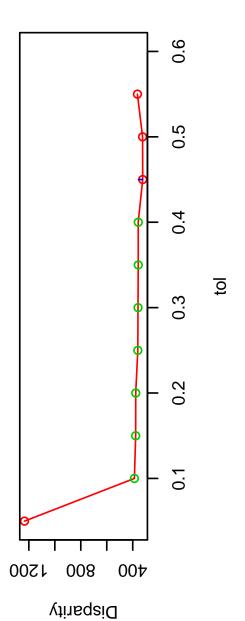


Fig. 3: Disparity against tol for 8 mass point model with unequal variances. Green circles: EM converged; red circles: EM not converged.

3.2 Compound Poisson models: The fabric faults data

In this Section we consider the fabric faults data, previously analyzed in Hinde (1982) and Aitkin, Francis & Hinde (2005, p. 453ff). This data describes the number of faults in rolls of fabrics with a single covariate leng for the length of the roll. The log-length is directly given by the variable x. The number of faults y can be assumed to follow a Poisson distribution. First, we fit a generalized linear Poisson model with the natural log link

```
Call: glm(formula = y ~ x, family = poisson(link = log), data = fabric)
                                                                              Call: glm(formula = y ~ 1, family = poisson(link = log), data = fabric)
                           > (faults0 <- glm(y ~ 1, family = poisson(link = log), data = fabric))
                                                                                                                                                                                                                                                                                                                                                                          > (faults1 <- glm(y ~ x, family = poisson(link = log), data = fabric))
                                                                                                                                                                                                                                                              Degrees of Freedom: 31 Total (i.e. Null); 31 Residual
                                                                                                                                                                                                                                                                                                                        AIC: 229
                                                                                                                                                                                                                                                                                        103.7
                                                                                                                                                                                                                                                                                                                         Residual Deviance: 103.7
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 0.997
                                                                                                                                                                                                                                                                                              Null Deviance:
> data(fabric)
                                                                                                                                         Coefficients:
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       Coefficients:
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               -4.173
                                                                                                                                                                                                   2.183
                                                                                                                                                                     (Intercept)
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   (Intercept)
```

Degrees of Freedom: 31 Total (i.e. Null); 30 Residual

103.7

AIC: 191.8

Residual Deviance: 64.54

Null Deviance:

and observe a large reduction in deviance by including the log length. Fits of count data with Poisson models are often quite poor, as the to model the unexplained variation by means of a Gaussian random effect Z. In case of the fabric fault data, one assumes that the number basic assumption underlying a Poisson model, equality of mean and variance, is often not adequate. As a solution, Hinde (1982) proposed of faults conditional on the observation and on the random effect follows a Poisson distribution, i.e.

$$Y|X_1,\ldots,X_n,Z\sim Po(\mu),$$

where $Z \sim N(0, 1)$, and

$$log(\mu) = c + log(leng) + \sigma Z,$$

Integrating out the random effect as in (1), one obtains a Poisson/normal compound distribution, which can be approximated with Gaussian quadrature (GQ). For one, two and three mass points one obtains with the log length as covariate:

```
> (faults.g1 <- alldist(y ~ x, family = poisson(link = log), random = ~1,
+ data = fabric, k = 1, random.distribution = "gq"))</pre>
```

data = fabric, k = 1, random.distribution = "gq") Call: alldist(formula = y ~ x, random = ~1, family = poisson(link = log),

Coefficients:

(Intercept)

×

-4.173 0.997

Random effect distribution - standard deviation:

0

-2 log L: 187.8

> (faults.g2 <- alldist(y ~ x, family = poisson(link = log), random = ~1,
+ data = fabric, k = 2, random.distribution = "gq"))</pre>

1 ..2 ..3 ..4 ..5 ..6 ..

EM algorithm met convergence criteria at iteration #

9

Disparity trend plotted.

data = fabric, k = 2, random.distribution = "gq") Call: alldist(formula = y ~ x, random = ~1, family = poisson(link = log),

Coefficients:

(Intercept)

0.3391 1.0331 0.3391081 Random effect distribution - standard deviation:

175.6 -2 log L: > (faults.g3 <- alldist(y ~ x, family = poisson(link = log), random = ~1,

data = fabric, k = 3, random.distribution = "gq", verbose = F)

data = fabric, k = 3, random.distribution = "gq", verbose Call: alldist(formula = y ~ x, random = ~1, family = poisson(link = log),

Coefficients:

(Intercept)

0.3575 0.8488 -3.3089 0.3574909 Random effect distribution - standard deviation:

174.3 -2 log L: The one mass point model is equivalent to the model faults1 given above, which can also be verified by checking the deviance

> faults.g1\$dev

[1] 64.53719

constant (the double saturated likelihood), which in our case takes the value 123.30. Thus, the disparity 174.3 for three mass points corresponds exactly to the deviance value of 51.0 reported in Hinde (1982), p. 119. For comparison, one can also fit the two and three For a Poisson model, deviance and disparity are related by the equation $D = Disp + 2L_{sat}$ and are consequently equal up to an additive mass point models with NPML:

```
data = fabric, k = 3, random.distribution = "np", verbose
                                                                                                                                                                                                                                                                                   data = fabric, k = 2, random.distribution = "np")
                                                                                                                 1 ..2 ..3 ..4 ..5 ..6 ..7 ..8 ..9 ..10 ..11 ..12 ..13 ..14 ..15 ..16 ..17 ..18 ..19 ..20 ..21 ..22 ..
                                                                                                                                                                                                                                                                                 Call: alldist(formula = y ~ x, random = ~1, family = poisson(link = log),
Call: alldist(formula = y ~ x, random = ~1, family = poisson(link = log),
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           > (faults.np3 <- alldist(y \tilde{} x, family = poisson(link = log), random = \tilde{}1,
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          data = fabric, k = 3, random.distribution = "np", verbose = FALSE))
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    0.3084855
                                                                                                                                                EM algorithm met convergence criteria at iteration # 22
                                                          data = fabric, k = 2, random.distribution = "np"))
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      Random effect distribution - standard deviation:
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  MASS3
                                                                                                                                                                                                                                                                                                                                                                               MASS2
                                                                                                                                                                                                                                                                                                                                                                                                               -2.4017
                                                                                                                                                                                  Disparity trend plotted.
                                                                                                                                                                                                                  EM Trajectories plotted.
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  MASS2
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       Mixture proportions:
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    0.7940023 0.2059977
                                                                                                                                                                                                                                                                                                                                                                                                                 0.8045 -3.1645
                                                                                                                                                                                                                                                                                                                                                                                     MASS1
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  MASS1
                                                                                                                                                                                                                                                                                                                                                    Coefficients:
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 Coefficients:
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          23
```

-3.114

0.798 -3.154

Random effect distribution - standard deviation:

0.307822

Mixture proportions:

MASS1 MASS2 MASS3 319235 0.6666708 0.2014057

0.1319235 0.6666708 0.201⁴ -2 log L: 172.7

from a normal distribution. While three mass points seem to be adequate for GQ, only two mass points are needed with NPML. Note that the use of option random.distribution="np" yields an object of type glmmNPML, while option random.distribution="gq" yields The disparities are not far from those obtained with Gaussian quadrature, indicating that the random effect distribution is not very far an object of type glmmGQ.

Predictions for objects of type \mathtt{glmmGQ} can be obtained by

```
> predict(faults.g2, type = "response", newdata = fabric[1:6, ])
```

1 2 3 4 5 6 8.7158 10.3546 13.3412 5.8568 11.4078 13.9380

.

> predict(faults.g2, type = "response")[1:6]

1 2 3 4 5 6 6.5578 7.0462 17.0202 7.2890 13.9926 9.5338

in the second case in an empirical Bayes approach (Aitkin, 1996a) using the individual posterior probabilities obtained as a by-product of which both call function predict.glmmGQ. The results of the two predictions differ, since in the first case prediction is done using the analytical mean of the marginal distribution, considering faults[1:6,] as 'new' input data (Aitkin, Hinde & Francis, 2005, p. 459), and the EM algorithm.

3.3 Logistic regression with random effects: The toxoplasmosis data

The toxoplasmosis data, also called rainfall data, are available via

```
> data(rainfall, package = "forward")
                                    > rainfall$x <- rainfall$Rain/1000
                                                                          > rainfall$x2 <- rainfall$x^2
                                                                                                                 > rainfall$x3 <- rainfall$x^3
```

x in 1000 mm. The data have been analyzed in Efron (1998) using generalized linear models and in Aitkin & Francis (1995) using the gives the number of subjects Cases out of Total testing positively for toxoplasmosis in each of 34 cities in El Salvador with annual rainfall

```
family = binomial(link = logit), data = rainfall, k =
GLIM 4 implementation of NPML. Fitting, as the latter authors, a constant logistic overdispersion model with three mass points, one
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 Call: alldist(formula = cbind(Cases, Total - Cases) ~ 1, random = ~1,
                                                                                                                                                       \tilde{1},
                                                                                                                                                > (toxo.np <- alldist(cbind(Cases, Total - Cases) ~ 1, random =</pre>
                                                                                                                                                                                                              data = rainfall, k = 3, family = binomial(link = logit)))
                                                                                                                                                                                                                                                                                                                                                                             EM algorithm met convergence criteria at iteration #
                                                                                                                                                                                                                                                                                                                   1 ..2 ..3 ..4 ..5 ..6 ..7 ..8 ..9 ..10 ..11 ..12 ..
                                                                                                                                                                                                                                                                                                                                                                                                                                       Disparity trend plotted.
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             EM Trajectories plotted.
```

3

Coefficients:

0.7615 0.1492 -0.9793 0.5996584 Random effect distribution - standard deviation:

Mixture proportions:

MASS1 MASS2 MASS3 0.33421659 0.57062599 0.09515743

-2 log L: 146.9

The result is approximately the same as that obtained by Aitkin & Francis (1995). However, note that the disparity

> toxo.np\$disparity

[1] 146.8668

differs from the GLIM 4 result 947.89. The disparity for binomial models provided by GLIM 4 has to be interpreted as $-2\log L + c$, where c is some additive constant only depending on the values of y and n, while the disparity given by this R implementation is just $-2 \log L$. Adding rainfall as fixed effect, we fit a linear random effect model

```
> (toxo.npx <- alldist(cbind(Cases, Total - Cases) ~ x, random = ~1,
+ data = rainfall, k = 3, family = binomial(link = logit)))</pre>
```

1 ..2 ..3 ..4 ..5 ..6 ..7 ..8 ..9 ..10 ..11 ..12 .. EM algorithm met convergence criteria at iteration # 12

Disparity trend plotted. EM Trajectories plotted. Call: alldist(formula = cbind(Cases, Total - Cases) ~ x, random = ~1,

family = binomial(link = logit), data = rainfall, k = 3)

Coefficients:

x MASS1 MASS2 MASS3 0.2897 -1.5494 -0.4063 0.2385 Random effect distribution - standard deviation: 0.6059427

Mixture proportions:

0.0890579 0.5787877 0.3321544

-2 log L:

The decrease in disparity compared to the constant model is only 0.3 on 1df (and is 5.1 for a cubic model, on 3df). We also try a random

> (toxo.npxx <- alldist(cbind(Cases, Total - Cases) ~ x, random = ~x,</pre>

data = rainfall, k = 3, family = binomial(link = logit)))

1 ..2 ..3 ..4 ..5 ..6 ..7 ..8 ..9 ..10 ..11 ..12 ..

EM algorithm met convergence criteria at iteration #

Disparity trend plotted.

EM Trajectories plotted.

Call: alldist(formula = cbind(Cases, Total - Cases) ~ x, random = ~x,

3

family = binomial(link = logit), data = rainfall, k =

Coefficients:

MASS3 MASS1:x MASS2:x MASS2 MASS1

1.1590 0.3038 2.0048 -0.7948 -0.6688 -0.2451

0.8089833 Random effect distribution - standard deviation:

Mixture proportions:

0.56715671 0.09714415 0.33569914

giving only a negligible decrease in disparity compared to the linear fixed effects model. All in all, when accounting for overdispersion, there is no overwhelming evidence that rainfall has a significant influence on the incidence of toxoplasmosis at all.

For the simple constant model, the posteriori probabilities w_{ik}

```
    16
    17
    18
    19
    20
    21
    22
    23
    24
    25
    26
    27
    28
    29
    30
    31

    1
    0.08
    0.45
    0.00
    0.01
    0
    0.01
    0.02
    0.00
    0.01
    0.00
    0.00
    0.00
    0.00

    2
    0.83
    0.49
    0.86
    0.69
    0.12
    0.07
    0.49
    0.73
    1
    0.99
    0.75
    0.99
    0.75
    0.98
    0.07
    0.83

                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             0.09\ 0.06\ 0.14\ 0.05\ 0.00\ 0.00\ 0.06\ 0.27\quad 0\ 0.00\ 0.02\ 0.01\ 0.24\ 0.02\ 0.93\ 0.14
                                                                                                                                                                                                                                                                                                          2 0.67 0.35 0.35 0.35 0.70 0.74 0.30 0.46 0.71 0.65 0.08 0.49 0.96 0.01 0.49
                                                                                                                                                                                                                                                                                                                                                                                                       3 0.09 0.01 0.02 0.01 0.19 0.12 0.01 0.00 0.08 0.35 0.00 0.06 0.02 0.00 0.06
                                                                                                                                                                                                                         1 0.25 0.64 0.63 0.64 0.11 0.14 0.69 0.53 0.21 0.00 0.92 0.45 0.02 0.99 0.45
     II
> round(t(toxo.np$post.prob), digits
```

mass point. From the posteriori probabilities, one also obtains the empirical Bayes predictions $\tilde{\eta}_i = \sum_k \hat{\eta}_{ik} \hat{w}_{ik}$ as in Aitkin (1996b), from which the predicted toxoplasmosis incidence probabilities $\tilde{p}_i = \exp(\tilde{\eta}_i)/(1 + \exp(\tilde{\eta}_i))$ can be calculated: show how the observations are allocated to the mass points, indicating that actually only one observation (the 30th) represents the 3rd

```
> round(toxo.ebp < toxo.np$ebp, digits = 3)
```

 1
 2
 3
 4
 5
 6
 7
 8
 9
 10
 11

 -0.079
 -0.566
 -0.555
 -0.566
 0.146
 0.065
 -0.622
 -0.450
 -0.041
 0.356
 -0.885

 12
 13
 14
 15
 16
 17
 18
 19
 20
 21
 22

 -0.326
 0.140
 -0.971
 -0.326
 0.114
 -0.326
 0.237
 -0.115
 -0.838
 -0.902
 -0.326

 23
 24
 25
 26
 27
 28
 29
 30
 31
 32
 33

0.304 0.152 0.139 -0.090 0.157 0.290 0.162 0.719 0.214 -0.566 -0.673

3 0.01 0.01 0.18 2 0.35 0.26 0.82

1 0.64 0.73 0.00

```
> round(exp(toxo.ebp)/(1 + exp(toxo.ebp)), digits = 4)

1 2 3 4 5 6 7 8 9 10 11

0.4803 0.3622 0.3647 0.3622 0.5363 0.5161 0.3494 0.3893 0.4899 0.5882 0.2921

12 13 14 15 16 17 18 19 20 21 22

0.4193 0.5350 0.2747 0.4193 0.5284 0.4193 0.5590 0.4714 0.3020 0.2886 0.4193

23 24 25 26 27 28 29 30 31 32 33

0.5754 0.5379 0.5347 0.4775 0.5393 0.5720 0.5403 0.6725 0.5534 0.3622 0.3378

34

0.5638
```

This can alternatively be done easier by using the generic predict function,

> fitted(toxo.np)

or, even quicker,

0.4802916 0.3621653 0.3646799 0.3621653 0.5363293 0.5161203 0.3493630 0.3893228 9 10 11 12 13

```
    17
    18
    19
    20
    21
    22
    23
    24

    0.4193273
    0.5589992
    0.4713726
    0.3019893
    0.2885689
    0.4193273
    0.5753992
    0.5378508

    25
    26
    27
    28
    29
    30
    31
    32

    0.5347178
    0.4775425
    0.5392603
    0.5719516
    0.5403452
    0.6724540
    0.55533823
    0.3621653

0.4898596\ 0.5881705\ 0.2920528\ 0.4193273\ 0.5350387\ 0.2747238\ 0.4193273\ 0.5283871
                                                                                                                                                                                                                                                                                                                                                                                                                                                                   0.3377802 0.5637801
```

which call function predict.glmmNPML for an object of type glmmNPML. The predict function can also be used to obtain predictions for new input values, e.g. for the linear random effect model:

```
> predict(toxo.npx, type = "response", newdata = data.frame(x = 2))
```

.

0.4628

3.4 Modelling mixtures of Gamma distributions: The hospital stay data

The hospital-stay data is a sample from a larger data set collected on persons discharged from a Pennsylvania hospital as part of a retrospective chart review of antibiotic use in hospitals (Rosner, 2000, p. 39). Relevant covariates of the data set are temp1 (the first measured temperature following admission, measured in Fahrenheit) and age, and the response is the duration of hospital stay. We read the data in and fit a three mass point model via

```
1 .. 2 .. 3 .. 4 .. 5 .. 6 .. 7 .. 8 .. 9 .. 10 .. 11 .. 12 .. 13 .. 14 .. 15 .. 16 .. 17 .. 18 .. 19 .. 20 .. 21 .. 22 .. 23 .. 24 .. 25 .. 26
                                                                                                                                                                                             EM algorithm met convergence criteria at iteration #
family = Gamma(link = log), tol = 0.2)
                                                                                                                                                                                                                                                            Disparity trend plotted.
```

> (fitnp3 <- alldist(duration ~ age + temp1, data = hosp, k = 3,

> data(hosp)

..27

EM Trajectories plotted.

data = hosp, k = 3, tol = 0.2) Call: alldist(formula = duration ~ age + temp1, family = Gamma(link = log),

Coefficients:

-32.369541 -33.021757 -33.801628 0.357537 temp1 age 0.004028

0.5069548 Random effect distribution - standard deviation:

Component distribution - MLE of shape parameter:

50.78

Mixture proportions:

MASS3 MASS2 MASS1

0.3980453 0.1220988 0.4798559

-2 log L:

giving the estimated shape parameter

> fitnp3\$shape

\$shape

[1] 50.78155

\$shapek

[1] 50.78155 50.78155 50.78155

(Certainly, all three component shape parameters listet at \$shapek are equal, as by default all components are assumed to have the same dispersion parameter.) For comparison, a three mass point mixture of exponentials (i.e. shape=1) is significantly inferior, yielding

> (fitnp3e <- alldist(duration ~ age + temp1, data = hosp, k = 3,

family = Gamma(link = log), to log(link = log)

```
..28 ..29 ..30
1 .. 2 .. 3 .. 4 .. 5 .. 6 .. 7 .. 8 .. 9 .. 10 .. 11 .. 12 .. 13 .. 14 .. 15 .. 16 .. 17 .. 18 .. 19 .. 20 .. 21 .. 22 .. 23 .. 24 .. 25 .. 26 .. 27
                                                                    41
                                                                EM algorithm met convergence criteria at iteration #
```

Disparity trend plotted.

EM Trajectories plotted.

data = hosp, k = 3, tol = 0.2, shape = 1) Call: alldist(formula = duration ~ age + temp1, family = Gamma(link = log),

Coefficients:

age temp1 MASS1 MASS2 MASS3 0.0149 0.3066 -28.6541 -28.6541 -28.6541

Component distribution - MLE of shape parameter: 1 Random effect distribution - standard deviation: 1.753596e-14

Mixture proportions:

MASS1 MASS2 MASS3 0.2295706 0.5465535 0.2238760

-2 log L: 155.2

For a more detailed analysis of this data set see Einbeck & Hinde (2006).

phenomenon occurs as the damping step modifies the likelihood, and hence the theoretical basis for EM is not given any more. Damped EM is actually only asymptotical EM, as for a large number of iterations the effect of damping vanishes. It depends on the application One important remark should still be given. When employing the damped EM algorithm, one will very occasionally observe rising and on tol what is a 'large' number of iterations. In general, rising disparities are more likely to be observed for small values of tol than for large values of tol, and more likely to be observed for Gamma than for Gaussian mixtures. Though these rising disparities are not really a problem, as at convergence the number of iterations is generally high enough, one might want to avoid them for esthetic reasons. disparities, typically from about the 10th to the 30th EM iteration. According to the theory on EM, this shouldn't happen.

This can be achieved by setting the constant damp.power in the formula

$$d_j = 1 - (1 - \mathtt{tol})^{\mathtt{damp.power*iter} + 1}$$

to a value bigger than one, where iter $\equiv j$ is the number of iterations and d_j is the multiplicative constant adjusting the dispersion parameter (Einbeck & Hinde, 2006). Another alternative is certainly to switch off damping (option damp=FALSE) but then it will not work at all in some cases.

3.5 Variance component models: The Oxford school boys data

This data set, also analyzed in Goldstein (2003), contains the heights of 26 boys in Oxford, measured on nine occasions over two years. The data set is contained in the R library nlme and can be loaded and plotted via

```
0000000000
                                                                                                                                                                                                          0
                                                                                                                                                                                     -0-
                                                                                                                            0
                                                                                                                                                                                                            0
                                                                                                                               0
                                             lines(Oxboys$age[Oxboys$boy == i], Oxboys$height[Oxboys$boy ==
i], pch = 1, type = "b", col = i)
                                                                                                                                                                                          0
                                                                                                                                                                                                              0
                                                                                                                                                                                                                                               0.5
                     1], ylim = c(125, 175), type = "b", pch = 1, xlab = "age", ylab = "height")
      > Oxboys$boy <- g1(26, 9)
> plot(Oxboys$age[Oxboys$boy == 1], Oxboys$height[Oxboys$boy ==
                                                                                                                                      \infty
                                                                                                                                                   0 ((() (() () () () () () () ()
                                                                                                                                                                                               0
                                                                                                                                                                                                                 0
                                                                                                                                                                       age
                                                                                                                                                                                                                                               0.0
                                                                                                                                                                                                                   0
                                                                                                                                              ||
|
|
|
                                                                                                                                                                                                                   0
                                     > for (i in 2:nlevels(Oxboys$Subject)) {
                                                                                                                                                    ||
|
|
|
                                                                                                                                                                                                                                               -0.5
                                                                                                                                                                                            000
                                                                                                                                                                                                                    0
> data(Oxboys, package = "nlme")
                                                                                                                                                        ..
დ
                                                                                                                                                                                                                      0
                                                                                                                                                                                                   000
                                                                                                                                                           00
                                                                                                                                                                                                                          0
                                                                                                                                                                      0۷١
                                                                                                                                                                    120
                                                                                                                                                                                                              130
```

height

Fig. 4: Oxford Boys Data

The boys represent the upper level (primary sampling units, PSU), and the particular measurements at different time points correspond to the lower-level units (secondary sampling units, SSU). Fitting a variance component model with Gaussian quadrature (20 mass points),

```
> (Oxboys.g20 <- allvc(height ~ age, random = ~1 | boy, data = Oxboys,</pre>
                                                                                                                                                                                 1 .. 2 .. 3 .. 4 .. 5 .. 6 .. 7 .. 8 .. 9 .. 10 .. 11 .. 12 .. 13 .. 14 .. 15
                                                                                                                                                                                                                                          EM algorithm met convergence criteria at iteration #
                                                     random.distribution = "gq", k = 20))
                                                                                                                                                                                                                                                                                        Disparity trend plotted.
                                                                                                                               [1] "1" "boy"
```

k = 20, random.distribution = "gq")

Coefficients:

Call: allvc(formula = height ~ age, random = ~1 | boy, data = Oxboys,

(Intercept) age z 148.958 6.524 4.769 Component distribution - MLE of sigma: 1.506 Random effect distribution - standard deviation:

4.76949

-2 log L: 991.8

out by Einbeck, Hinde & Darnell (2007). It turns out that a huge number of mass points $K \approx 500$ is needed in this example to get down This is no satisfactory solution since fitting the same data with function lmer in R package lme4 gives a disparity of 940.6, as pointed to a similar disparity. We have observed this phenomenon also at other occasions and it seems to occur only if the intra-class correlation (ICC), given by

$$ICC = \frac{\sigma_z^2}{\sigma_z^2 + \sigma^2}$$

is quite large. For example, for the model fitted above it is

> Oxboys.g20%rsdev^2/(Oxboys.g20%rsdev^2 + Oxboys.g20%sdev%sdev^2)

[1] 0.9093017

which is a very large value. We have not observed this problem for smaller ICCs, i.e. roughly $ICC \le 0.5$. Fortunately, the problem does not persist for NPML estimation. For illustration, we fit NPML with seven (as suggested by Aitkin, Hinde & Francis (2005), p. 495), and eight masspoints, yielding

```
> (Oxboys.np7 <- allvc(height ~ age, random = ~1 | boy, data = Oxboys,</p>
                                                                                                                                                              10
                                                                                                                                                              EM algorithm met convergence criteria at iteration #
                                          random.distribution = "np", k = 7))
                                                                                                                1 ..2 ..3 ..4 ..5 ..6 ..7 ..8 ..9 ..10 ..
```

Disparity trend plotted.

EM Trajectories plotted.

k = 7, random.distribution = "np") Call: allvc(formula = height ~ age, random = ~1 | boy, data = Oxboys,

Coefficients:

164.884 MASS6 159.521 155.261 MASS5 149.967 MASS4 144.605 138.417 MASS2 age MASS1 6.524 130.200 MASS1

1.762 Component distribution - MLE of sigma: 7.850653 Random effect distribution - standard deviation:

Mixture proportions:

MASS6 0.34544795 0.19228146 0.03846828 MASS5 MASS4 0.19303307 MASS3 0.11538462 0.03846154

MASS7

0.07692308

-2 log L:

```
k = 8, random.distribution = "np")
                                                                                                                                                                                                                                                                                                                                                                         Call: allvc(formula = height ~ age, random = ~1 | boy, data = Oxboys,
> (Oxboys.np8 <- allvc(height ~ age, random = ~1 | boy, data = Oxboys,</p>
                                                                                                                                                                             EM algorithm met convergence criteria at iteration # 10
                                            random.distribution = "np", k = 8))
                                                                                                                             1 ..2 ..3 ..4 ..5 ..6 ..7 ..8 ..9 ..10 ..
                                                                                                                                                                                                                            Disparity trend plotted.
                                                                                                                                                                                                                                                                            EM Trajectories plotted.
```

Coefficients: age MASS1 MASS2 MASS3 MASS4 MASS5 MASS6 MASS7 6.524 130.200 138.417 143.382 147.350 151.267 155.789 159.522 MASS8

Component distribution - MLE of sigma: 1.433

Random effect distribution - standard deviation: 7.917343

Mixture proportions:

 MASS1
 MASS2
 MASS3
 MASS4
 MASS5
 MASS6

 0.03846154
 0.11538462
 0.11538469
 0.19230765
 0.26921962
 0.15385725

 MASS7
 MASS8

 0.03846155
 0.07692308

 -2 log L:
 931.4

Thus, NPML with 8 mass points already leads to a better result than GQ with 20 mass points. The EM trajectories, as shown in Fig. 5, can also be obtained explicitly by calling

> plot(Oxboys.np8, plot.opt = 2)

164.884

We now extend the 8-point model by allowing the linear trend to vary across boys.

```
> (Oxboys.np8s <- allvc(height ~ age, random = ~age | boy, data = Oxboys,
+ random.distribution = "np", k = 8))</pre>
```

1 ..2 ..3 ..4 ..5 ..6 ..7 ..8 ..9 ..10 ..
EM algorithm met convergence criteria at iteration # 10
Disparity trend plotted.
EM Trajectories plotted.

k = 8, random.distribution = "np") Call: allvc(formula = height ~ age, random = ~age | boy, data = Oxboys,

Coefficients:

MASS6 155.7763 MASS5:age -2.5653 MASS4:age MASS5 151.2646 -3.7833 MASS3:age MASS4 147.3756 -2.1543MASS3 143.3707 MASS2:age -4.0056 MASS2 138.4476 MASS1:age -5.4901MASS1 130.2616 MASS8 164.8242 MASS7:age MASS7 MASS6:age 9.2130 159.4738

-0.5421

-2.1239

Component distribution - MLE of sigma:

Random effect distribution - standard deviation: 7.893352

1.185

Mixture proportions:

MASS1 MASS2 MASS3 MASS4 MASS5 MASS6 0.03846154 0.11538462 0.11538462 0.19230769 0.26923047 0.15384645

MASS7 MASS8

0.03846154 0.07692308

842.4

-2 log L:

The difference in disparities is

> Oxboys.np8\$disp - Oxboys.np8s\$disp

[1] 88.93035

on 7df, showing clear heterogeneity in the slope.

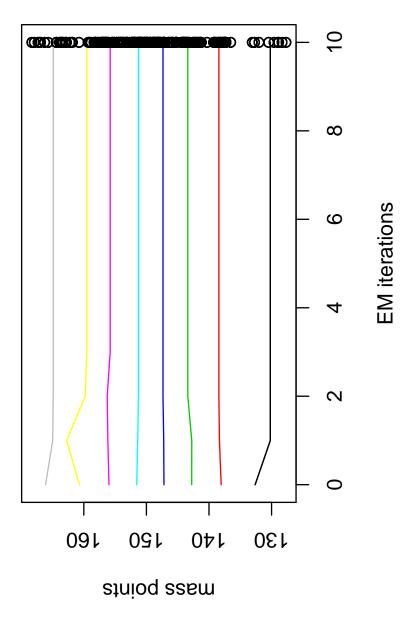


Fig. 5: Convergence of EM for eight mass points, applied on Oxford boys data.

3.6 Spatial random effect models: Irish Suicide Data

The data considered here, available in the package npmlreg via

> data(irlsuicide)

model with regions as cluster variable, categorical covariates for gender and age, interaction terms, and an offset representing the cluster sizes. The R code can be found in the Examples section of the help file for allvc (page 8 in the reference manual). While the random between regions is included into the model by employing an extra - fixed or random - covariate representing the average crude suicide describe the mortality due to suicide and intentional self-harm in the Republic of Ireland from 1989–1998. Suicide rates are modelled using either the average crude rate or the relative risk as model parameter. The analysis of these data involves a variance component effect accounts for within-region correlation, it is worthwile to consider between-region correlation in this application. Spatial correlation rates from the neighboring regions (or the average neighboring standard mortality ratios, respectively). For details, see Sofroniou, Einbeck and Hinde (2006).

4 Citation

The correct citation for R package npmlreg can be queried with

> citation(package = "npmlreg")

To cite package âĂŸnpmlregâĂŹ in publications use:

Jochen Einbeck, Ross Darnell and John Hinde (2009). npmlreg: Nonparametric maximum likelihood estimation for random effect models. R package version 0.44.

A BibTeX entry for LaTeX users is

@Manual{,

```
title = {npmlreg: Nonparametric maximum likelihood estimation for random effect models},
                                                                                                                                                                                                                                                                                                                   ATTENTION: This citation information has been auto-generated from the
                                                   author = {Jochen Einbeck and Ross Darnell and John Hinde},
                                                                                                                                                                                                                                                                                                                                                                      package DESCRIPTION file and may need manual editing, see
                                                                                                                                                            note = {R package version 0.44},
                                                                                                                                                                                                                                                                                                                                                                                                                         aĂŸhelp("citation")âĂŹ .
                                                                                                      year = {2009},
```

The correct citation for this R vignette is

EINBECK, J. and HINDE, J. (2009). Nonparametric maximum likelihood estimation for random effect models in R. Vignette to R. package **npmlreg** version 0.44.

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6 Appendix: R Documentation

A printed version of the help files is available in the reference manual, which can be downloaded from CRAN at

http://cran.r-project.org/src/contrib/Descriptions/npmlreg.html.

A list of all functions currently availabe in **npmlreg** is given below:

> ls("package:npmlreg")

"binomial.expand" "print.glmmNPML" "tolfind" "predict.glmmGQ" "model.matrix.glmmNPML" "plot.glmmGQ" "expand.vc" "gqz" "family.glmmNPML" "print.glmmGQ" "expand" "allvc" "post" [10] "model.matrix.glmmGQ" [16] "predict.glmmNPML" [13] "plot.glmmNPML" [7] "family.glmmGQ" [1] "alldist" [4] "dkern"

In addition, the data sets fabric, irlsucide, hosp, and missouri are available.

"summary.glmmNPML"

[22] "weightslogl.calc.w"

[19] "summary.glmmGQ"