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 approxmating the generalized linear models with random effects was previously implemented by Aitkin & Francis (1995) in the GLIM4 language, which is marginal likelihood by a simple finite mixture, for which standard fitting algorithms based on EM exist and can be applied. NPML for however no longer widely used. The main functions of this package, alldist (for overdispersion) and allvc (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 Ross Darnell.

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

http://cran.r-project.org.

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

distribution¹ $f(y_i|\beta,\phi_i)$ with dispersion parameter ϕ_i . In a generalized linear model, predictors and response are assumed to be related 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 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 $Var(y_i|\beta,\phi_i) = \phi_i v(\mu_i)$ 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, Gamma and Inverse Gaussian 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

$$\prod_{i=1}^n \left\{ \sum_{k=1}^K f(y_i | z_k, \beta, \phi_k) \pi_k \right\} \equiv \prod_{i=1}^n \left\{ \sum_{k=1}^K f_{ik} \pi_k \right\},$$

where z_k are the mass points and π_k their masses. The log-likelihood is then given by

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$$\ell = \sum_{i=1}^{n} \log\left\{\sum_{k=1}^{K} \pi_k f_{ik}\right\}.$$
(2)

The score equations

$$\frac{\partial \ell}{\partial z_k} = 0, \quad \frac{\partial \ell}{\partial \beta} = 0, \quad \frac{\partial \ell}{\partial \phi_k} = 0, \tag{3}$$

turn out to be weighted versions of the single-distribution score equations, with weights

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

$$\hat{\tau}_k = \frac{1}{n} \sum_i w_{ik} \tag{5}$$

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 $\pi_k^{(0)}$, $k = 1, \ldots, K$.

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. 5

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 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 (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 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)

3 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 The data considered in this example are the recession velocities (in km/s) of 82 galaxies receding from our own, sampled from six wellseparated 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 obtain 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 $10^3 km/s$:

> gal\$v1000<- gal\$galaxies/1000</pre>

6

> gal\$v1000

23.711 32.065 21.960 9.775 10.227 10.406 16.084 16.170 18.419 18.552 18.600 18.927 19.052 19.070 19.330 19.343 19.349 19.440 19.473 19.529 19.541 19.547 19.663 19.846 19.856 19.863 19.914 19.918 19.973 20.215 20.221 20.415 20.629 20.795 22.888 26.995 21.814 21.921 22.495 22.746 22.747 23.666 23.706 26.960 21.701 23.542 25.633 23.538 24.990 21.49222.374 20.179 20.196 22.249 22.314 23.263 23.484 24.366 24.717 20.875 20.986 21.137 9.558 9.350 9.483 20.175 22.242 23.241 24.289 19.989 20.166 20.846 22.209 23.206 24.285 9.172 22.914 20.821 22.185 24.129 Ξ [11][21] [31] [41] [51][61][71]

and load the **npmlreg** package:

34.279

32.789

81]

> library(npmlreg)

Fitting a simple constant normal model yields

> glm(v1000~1,data=gal)

Call: glm(formula = v1000 ~ 1, data = gal)

Coefficients: (Intercept) 20.83 Degrees of Freedom: 81 Total (i.e. Null); 81 Residual Null Deviance: 1690 Residual Deviance: 1690 AIC: 484.8

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which is the same as a NPML estimation with one mass point, fitting a 'mixture' of one normal component:

> (galaxy.np1 <- alldist(v1000~1,random=~1,random.distribution='np',k=1,data=gal))</pre>

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

Coefficients: MASS1 20.83 Component distribution - MLE of sigma: 4.568 Random effect distribution - standard deviation: 0

Mixture proportions:

MASS1 1 -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))</p>

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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 37 EM algorithm met convergence criteria at iteration # Disparity trend plotted. EM Trajectories plotted.

random.distribution = "np") Call: alldist(formula = $v1000 \sim 1$, 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

Mixture proportions:

random.distribution = "np") > (galaxy.np3 <- alldist(v1000~1,random=~1,random.distribution='np',k=3,data=gal))</p> > (galaxy.np4 <- alldist(v1000~1,random=~1,random.distribution='np',k=4,data=gal))</p> 1 ..2 ..3 ..4 ..5 ..6 ..7 ..8 ..9 ..10 ..11 ..12 ..13 ..14 ..15 ..16 ..17 ..18 .. Call: alldist(formula = v1000 ~ 1, random = ~1, data = gal, k = 3, 4.03618 EM algorithm met convergence criteria at iteration # 18 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 425.4 461Disparity trend plotted. Disparity trend plotted. EM Trajectories plotted. MASS2 MASS2 0.91305867 Mixture proportions: MASS1 MASS2 MASS3 32.94 21.40Coefficients: 0.08694133 MASS1 MASS1 -2 log L: -2 log L: 9.75

EM Trajectories plotted.

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

Coefficients: MASS1 MASS2 MASS3 MASS4 9.71 20.00 23.50 33.04 Component distribution - MLE of sigma: 1.315 Random effect distribution - standard deviation: 4.345212

Mixture proportions: MASS1 MASS2 MASS3 MASS4 0.08536797 0.52624187 0.35180277 0.03658738 -2 log L: 416.5

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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).





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</pre>

[1] 410.6852

> (galaxy.np6 <- alldist(v1000~1,random=~1,k=6,tol=0.2,data=gal,verbose=FALSE))\$disp</pre>

[1] 394.5811

> (galaxy.np7 <- alldist(v1000~1,random=~1,k=7,tol=0.12,data=gal,verbose=FALSE))\$disp</pre>

[1] 388.8639

> (galaxy.np8 <- alldist(v1000~1,random=~1,k=8,tol=0.2,data=gal,verbose=FALSE))\$disp</pre>

[1] 388.177

> (galaxy.np9 <- alldist(v1000~1,random=~1,k=9,tol=0.06,data=gal,verbose=FALSE))\$disp</pre>

[1] 388.2149

mean 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 indicating that the disparity stabilizes at about 8 mass points. Note that in some cases it was necessary to modify the optional parameter tol to obtain the disparity values given above. The tol parameter influences the position of the starting points, where values tol < 1is less sensitive to the optimal choice of to1, the optimal solutions are found more easily. An assisting tool in the selection of to1 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

$$V(x,y|\lambda) = \begin{cases} \lambda & \text{if } y = x \\ (1-\lambda)/(K-1) & \text{if } y \neq x \end{cases}$$

(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 $1/K \leq \lambda \leq 1$. 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(v1000~1, random=~1, k=4, tol=0.5, data=gal, lambda=1, verbose=FALSE))</pre>

tol = 0.5, lambda = 1, verbose = FALSE) Call: alldist(formula = $v1000 \sim 1$, random = ~ 1 , data = gal, k = 4,

Coefficients:

Estimate Std. Error ASS1 9.710143 0.2776675 ASS2 19.949549 0.1174379 ASS3 23.135282 0.1281410) 180.54545 77 00005	30806.77 8
Estimate ASS1 9.710143 ASS2 19.949549 ASS3 23.135282	0.1281410	0.4241455
ASS1 ASS2 ASS3	23.135282	33.044336
$\Sigma \Sigma \Sigma$	MASS3	MASS4

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: 4.302845

-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 of unequal component dispersion parameters, as the the disparity does not share this problem. This is also the reason why we prefer to An important remark should be given here: Interpretation (and definition!) of the deviance $D = -2\phi \log L + 2\phi \log L_{saturated}$, 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 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
<pre>Error in alldist(v1000 1, random = 1, k = 8, tol = 0.5, data = gal, : Singularity or Likelihood-Spike at iteration #12. Check model specification, enable spike protection or smooth among components.</pre>
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 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 enable the spike protection (spike.protect=1), which stops the algorithm as soon as one component starts to enter a likelihood spike.
> (galaxy.np8us <- alldist(v1000~1, random=~1, k=8, tol=0.5, data=gal, lambda=1, verbose=FALSE, spike.protect=TRUE))
Call: alldist(formula = v1000 ~ 1, random = ~1, data = gal, k = 8, tol = 0.5, lambda = 1, spike.protect = TRUE, verbose = FALSE)
Coefficients: MASS1 MASS2 MASS3 MASS4 MASS5 MASS6 MASS7 MASS8 9.383 9.906 17.233 19.772 22.587 24.410 32.433 34.279
Random effect distribution - standard deviation: 4.417512
Mixture proportions: MASS1 MASS2 MASS3 MASS4 MASS5 MASS6 0.03457724 0.05078828 0.03637014 0.37478549 0.35365507 0.11323979 MASS7 MASS8 0.02438886 0.01219512 -2 log L: 220
> galaxy.np8us\$sdev\$sdevk

<pre>[1] 1.504988e-01 4.113445e-01 1.526060e+00 6.309877e-01 1.170915e+00 [6] 1.738375e+00 3.757823e-01 2.645245e-37</pre>	gives us estimates of mass points, masses, and standard deviations of the mixture components. These values have to be interpreted with care, as the displayed disparity is normally not correct when the algorithm does not have converged. One notices from this output that 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:	<pre>> (galaxy.np8ud <- alldist(v1000~1, random=~1, k=8, tol=0.5, data=gal, lambda=0.99))</pre>	1234567891011121314151617181920212223242526272829 EM algorithm met convergence criteria at iteration # 102 Disparity trend plotted. EM Trajectories plotted.	Call: alldist(formula = v1000 ~ 1, random = ~1, data = gal, k = 8, tol = 0.5, lambda = 0.99)	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 MASS5 7.888540e-15 8.536585e-02 2.439018e-02 4.039238e-01 4.256102e-01 MASS6 MASS7 MASS8 0.410464a-00 1.040446-00
--	--	---	---	--	---	---	--

> 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 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 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 should consequently be chosen from them.

> par(mfrow=c(1,1), cex=0.65)

> tolfind(v1000~1, random=~1, k=8, data=gal, lambda=1, find.in.range=c(0.0,0.6), steps=12, plot.opt=0, verbose=FALSE, noformat=TRUE)[c(

357.8221 360.9393 359.4521 Minimal Disparity with EM converged: 357.8216 at tol= 0.4 377.0345 363.8772 Minimal Disparity: 219.9949 at tol= 0.5 377.6917 219.9949 [1] 1233.6883 387.2360 \$AllDisparities

Inf [8] 357.8216 323.3126

\$Alltol

[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



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

> data(fabric)

```
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))</pre>
                                                                                                                                                                                                                                                                                                                                          > (faults1 <- glm(y ~ x, family=poisson(link=log),data=fabric))</pre>
                                                                                                                                                                                                                                Degrees of Freedom: 31 Total (i.e. Null); 31 Residual
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        Degrees of Freedom: 31 Total (i.e. Null); 30 Residual
                                                                                                                                                                                                                                                                                         AIC: 229
                                                                                                                                                                                                                                                            103.7
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       103.7
                                                                                                                                                                                                                                                                                           Residual Deviance: 103.7
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       ×
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               0.9969
                                                                                                                                                                                                                                                               Null Deviance:
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       Null Deviance:
                                                                                                               Coefficients:
                                                                                                                                                                                                                                                                                                                                                                                                                                                      Coefficients:
                                                                                                                                                                      2.183
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               -4.1730
                                                                                                                                         (Intercept)
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  (Intercept)
```

AIC: 191.8

Residual Deviance: 64.54

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 pasic assumption underlying a Poisson model, equality of mean and variance, is often not adequate. As a solution, Hinde (1982) proposed 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 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"))
Call: alldist(formula = y ~ x, random = ~1, family = poisson(link = log), data = fabric, k = 1, random.distribution = "gq")
Coefficients: (Intercept) x -4.1730 0.9969 Aandom 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"))
l23456 EM algorithm met convergence criteria at iteration # 6 Disparity trend plotted.
Call: alldist(formula = y ~ x, random = ~1, family = poisson(link = log), data = fabric, k = 2, random.distribution = "gq")

data = fabric, k = 3, random.distribution = "gq", verbose > (faults.g3<- alldist(y ~ x, family=poisson(link=log), random=~1, data= fabric,k=3, random.distribution="gq",verbose=F))</pre> Call: alldist(formula = y ~ x, random = ~1, family = poisson(link = log), 0.3574909 0.3391081 Random effect distribution - standard deviation: Random effect distribution - standard deviation: Ν Ν 0.3575 0.3391 175.6 174.3 × × 1.0331 0.8488 Coefficients: Coefficients: -3.3089-4.4128(Intercept) (Intercept) -2 log L: -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

22

[1] 64.53719

For a Poisson model, deviance and disparity are related by the equation $D = Disp + 2L_{sat}$ and are consequently equal up to an additive 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 mass point models with NPML:

> (faults.np2<- alldist(y ~ x, family=poisson(link=log), random=~1, data= fabric,k=2, random.distribution="np"))</p>

12345678910111213141516171819 . EM algorithm met convergence criteria at iteration # 22 Disparity trend plotted. EM Trajectories plotted.	202122
<pre>Call: alldist(formula = y ~ x, random = ~1, family = poisson(link = log), data</pre>	<pre>L = fabric, k = 2, random.distribution = "np")</pre>
Coefficients: x MASS1 MASS2 0.8045 -3.1645 -2.4017	
Random effect distribution - standard deviation: 0.3084855	
Mixture proportions: MASS1 MASS2 0.7940023 0.2059977 -2 log L: 172.7	
<pre>> (faults.np3<- alldist(y ~ x, family=poisson(link=log), random=~1, data= fabric,k=3,</pre>	<pre>3, random.distribution="np",verbose=FALSE))</pre>
Call: alldist(formula = y ~ x, random = ~1, family = poisson(link = log), data	<pre>l = fabric, k = 3, random.distribution = "np", verbose</pre>
Coefficients: x MASS1 MASS2 MASS3 0.798 -3.154 -3.114 -2.353	
Random effect distribution - standard deviation: 0.307822	

Mixture proportions:

```
MASS1 MASS2 MASS3
0.1319235 0.6666708 0.2014057
-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 The disparities are not far from those obtained with Gaussian quadrature, indicating that the random effect distribution is not very far that the use of option random.distribution="np" yields an object of type glmmNPML, while option random.distribution="gq" yields an object of type glmmGQ.

Predictions for objects of type 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
```

24

or

```
> 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
```

which both call function predict.glmmGQ. The results of the two predictions differ, since in the first case prediction is done using the in the second case in an empirical Bayes approach (Aitkin, 1996a) using the individual posterior probabilities obtained as a by-product analytical mean of the marginal distribution, considering faults[1:6,] as 'new' input data (Aitkin, Hinde & Francis, 2005, p. 459), and of 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) > rainfall\$x<-rainfall\$Rain/1000 > rainfall\$x2<- rainfall\$x^2; rainfall\$x3<- rainfall\$x^3
gives the number of subjects Cases out of Total testing positively for toxoplasmosis in each of 34 cities in El Salvador with annual rainfall x in 1000 mm. The data have been analyzed in Efron (1998) using generalized linear models and in Aitkin & Francis (1995) using the GLIM 4 implementation of NPML. Fitting, as the latter authors, a constant logistic overdispersion model with three mass points, one obtains
> (toxo.np<- alldist(cbind(Cases,Total-Cases)~1, random=~1, data=rainfall, k=3, family=binomial(link=logit)))
123456789101112 EM algorithm met convergence criteria at iteration # 12 Disparity trend plotted. EM Trajectories plotted.
Call: alldist(formula = cbind(Cases, Total - Cases) ~ 1, random = ~1, family = binomial(link = logit), data = rainfall, k = 3)
Coefficients: MASS1 MASS2 MASS3 -0.9793 0.1492 0.7615
Random effect distribution - standard deviation: 0.5996584
Mixture proportions: MASS1 MASS2 MASS3 0.33421659 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

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 \mathbf{y} and \mathbf{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)))
123456789101112 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: MASS1 MASS2 MASS3 0.33215441 0.578769 0.08905789 -2 log L: 146.6
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 slope

> toxo.np\$disparity

[1] 146.8668

123456789101112 EM algorithm met convergence criteria at iteration # 12 Disparity trend plotted. EM Trajectories plotted.
Call: alldist(formula = cbind(Cases, Total - Cases) ~ x, random = ~x, family = binomial(link = logit), data = rainfall, k = 3)
Coefficients: x MASS1 MASS2 MASS3 MASS1:x MASS2:x -0.6688 -0.2451 -0.7948 2.0048 0.3038 1.1590
Random effect distribution - standard deviation: 0.8089833
Mixture proportions: MASS1 MASS2 MASS3 0.33569914 0.56715671 0.09714415 -2 log L: 146.1
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}
<pre>> round(t(toxo.np\$post.prob),digits=2)</pre>
$\begin{array}{cccccccccccccccccccccccccccccccccccc$

(toxo.npxx<- alldist(cbind(Cases,Total-Cases)~x, random=~x, data=rainfall, k=3, family=binomial(link=logit)))

^

```
3 0.09 0.06 0.14 0.05 0.00 0.00 0.06 0.27 0 0.00 0.02 0.01 0.24 0.02 0.93 0.14
                                                                  1 0.64 0.73 0.00
2 0.35 0.26 0.82
                                                      34
                                                      33
                                                      32
```

show how the observations are allocated to the mass points, indicating that actually only one observation (the 30th) represents the 3rd mass point. From the posteriori probabilites, 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:

> round(toxo.ebp<-toxo.np\$ebp,digits=3)</pre>

3 0.01 0.01 0.18

11	-0.885	22	-0.326	33	-0.673		
10	0.356	21	-0.902	32	-0.566		
თ	-0.041	20	-0.838	31	0.214		
00	-0.450	19	-0.115	30	0.719		
7	-0.622	18	0.237	29	0.162		
9	0.065	17	-0.326	28	0.290		
വ	0.146	16	0.114	27	0.157		
4	-0.566	15	-0.326	26	-0.090		
n	-0.555	14	-0.971	25	0.139		
7	-0.566	13	0.140	24	0.152		
	0.079	12	0.326	23	0.304	34	0.257

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

 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

0.5638

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

> predict(toxo.np, type="response")

0.5638

or, even quicker,

> fitted(toxo.np)

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))

1 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

> data(hosp)

30

> (fitnp3<- alldist(duration~age+temp1, data=hosp,k=3, family=Gamma(link=log),tol=0.2))</pre>

: 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 27 EM algorithm met convergence criteria at iteration # Disparity trend plotted. EM Trajectories plotted.

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

Coefficients:

age temp1 MASS1 MASS2 MASS3 0.004028 0.357537 -33.801628 -33.021757 -32.369541 Component distribution - MLE of shape parameter: 50.78

Random effect distribution - standard deviation:

0.5069548

Mixture proportions: MASS1 MASS2 MASS3 0.4798559 0.3980453 0.1220988 -2 log L: 121.3

giving the estimated shape parameter

> fitnp3\$shape

\$shape [1] 50.78155 \$shapek [1] 50.78155 50.78155 50.78155

31

(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

(fitup3e<- alldist(duration~age+temp1, data=hosp,k=3, family=Gamma(link=log),tol=0.2,shape=1)) ^

 $1 \dots 2 \dots 3 \dots 4 \dots 5 \dots 6 \dots 7 \dots 8 \dots 9 \dots 10 \dots 11 \dots 12 \dots 13 \dots 14 \dots 15 \dots 16 \dots 17 \dots 18 \dots 19 \dots 20 \dots 21 \dots 23 \dots 24 \dots 25 \dots 26 \dots 27 \dots 29 \dots 30$ EM algorithm met convergence criteria at iteration # 41 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 0.0149	temp1 0.3066	MASS1 -28.6541	MASS2 -28.6541	MASS3 - 28.6541	
)))			1 1))]	
Component	distribut	ion - MLE	of shape p	arameter:	1
Random efi	ect distr	ibution -	standard d	eviation:	3.118363e-15
Mixture pı	oportions	••			

	MASS3	0.2238760	155.2
4	MASS2	0.5465535	
•	MASS1	0.2295706	-2 log L:

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

ThisOne important remark should still be given. When employing the damped EM algorithm, one will very occasionally observe rising phenomenon occurs as the damping step modifies the likelihood, and hence the theoretical basis for EM is not given any more. Damped 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 EM is actually only asymptotical EM, as for a large number of iterations the effect of damping vanishes. It depends on the application 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

$$l_{i}=1-(1-\texttt{tol}){ t damp} \cdot \texttt{power} * \texttt{iter} + 1$$

to a value bigger than one, where $iter \equiv j$ is the number of iterations and d_i 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

- > data(Dxboys, package = "nlme")
 - > Uxboys\$boy <- g1(26,9)</pre>
- plot (0xboys \$age [0xboys \$boy = 1], 0xboys \$height [0xboys \$boy = 1], ylim = c(125, 175), type = 'b', pch = 1, xlab = 'age', ylab = 'height')^
- for (i in 2:nlevels(0xboys\$Subject)){lines(0xboys\$age[0xboys\$boy==i],0xboys\$height[0xboys\$boy==i], pch=1,type='b',col=i)} ~





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), one gets

(0xboys.g20 <- allvc(height~age,random=~1/boy,data=0xboys,random.distribution='gq',k=20)) ~

k = 20, random.distribution = "gq") Call: allvc(formula = height ~ age, random = ~1 | boy, data = Oxboys, : 1 ..2 ..3 ..4 ..5 ..6 ..7 ..8 ..9 ..10 ..11 ..12 ..13 ..14 ..15 15 EM algorithm met convergence criteria at iteration # Disparity trend plotted. Coefficients: (Intercept)

Component distribution - MLE of sigma: 1.506 Random effect distribution - standard deviation: 4.76949

z 4.769

age 6.524

148.958

-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

> Dxboys.g20\$rsdev^2/(Dxboys.g20\$rsdev^2+ Dxboys.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 $ICC \leq 0.5$. 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,random.distribution='np',k=7)) ~

k = 7, random.distribution = "np") Call: allvc(formula = height ~ age, random = ~1 | boy, data = Oxboys, MASS7 MASS6 10 EM algorithm met convergence criteria at iteration # **MASS5** MASS4 $1 \dots 2 \dots 3 \dots 4 \dots 5 \dots 6 \dots 7 \dots 8 \dots 9 \dots 10 \dots$ MASS3 MASS2 Disparity trend plotted. EM Trajectories plotted. MASS1 Coefficients: age

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

164.884

159.521

155.261

149.967

144.605

138.417

6.524 130.200

36

Mixture proportions: Mass1 MASS2 MASS3 MASS4 MASS5 MASS6 0.03846154 0.11538462 0.19303307 0.34544795 0.19228146 0.03846828 MASS7 0.07692308 -2 log L: 1017.3 > (0xboys.np8 <- allvc(height~age,random=~1/boy,data=0xboys,random.distribution='np',k=8))</p>

k = 8, random.distribution = "np") Call: allvc(formula = height ~ age, random = ~1 | boy, data = Oxboys, MASS7 159.522 MASS6 0.26921962 0.15385725 7.917343 MASS6 155.789 **MASS5** 10 1.433 EM algorithm met convergence criteria at iteration # **MASS5** 151.267 Random effect distribution - standard deviation: 0.11538462 0.11538469 0.19230765 MASS4 MASS4 147.350 1 ..2 ..3 ..4 ..5 ..6 ..7 ..8 ..9 ..10 .. Component distribution - MLE of sigma: 138.417 143.382 MASS3 **MASS3** 931.4 MASS2 Disparity trend plotted. EM Trajectories plotted. MASS8 MASS2 0.07692308 Mixture proportions: 6.524 130.200 MASS1 Coefficients: 0.03846154 0.03846155 MASS1 MASS7 -2 log L: age MASS8 164.884

37

ų 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. can also be obtained explicitly by calling

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

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

> (Dxboys.np8s <- allvc(height~age,random=~age/boy,data=Dxboys,random.distribution='np',k=8))</p>

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:

					-0.5421	-2.1239
					MASS7:age	MASS6:age
-2.5653	-3.7833	-2.1543	-4.0056	-5.4901	164.8242	159.4738
MASS5:age	MASS4:age	MASS3:age	MASS2:age	MASS1:age	MASS8	MASS7
155.7763	151.2646	147.3756	143.3707	138.4476	130.2616	9.2130
MASS6	MASS5	MASS4	MASS3	MASS2	MASS1	age

38

Component distribution - MLE of sigma: 1.185 Random effect distribution - standard deviation: 7.893352

Mixture proportions:

) 			2.4	0.07692308 84	MASS7 MASS7 3846154 log L:
				0.07692308	346154
				MASS8	MASS7
0.15384645	0.26923047	0.19230769	0.11538462	0.11538462	346154
MASS6	MASS5	MASS4	MASS3	MASS2	MASS1

The difference in disparities is

> 0xboys.np8\$disp-0xboys.np8s\$disp

[1] 88.93035

on 7df, showing clear heterogeneity in the slope.





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 using either the average crude rate or the relative risk as model parameter. The analysis of these data involves a variance component 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 effect accounts for within-region correlation, it is worthwile to consider between-region correlation in this application. Spatial correlation between regions is included into the model by employing an extra - fixed or random - covariate representing the average crude suicide rates from the neighboring regions (or the average neighboring standard mortality ratios, respectively). For details, see Sofroniou, Einbeck describe the mortality due to suicide and intentional self-harm in the Republic of Ireland from 1989–1998. Suicide rates are modelled and Hinde (2006).

4 Citation

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The correct citation for R package **npmlreg** can be queried with

> citation(package="npmlreg")

To cite package 'npmlreg' in publications use:

Einbeck J, Darnell R, Hinde J (2018). _npmlreg: Nonparametric Maximum Likelihood Estimation for Random Effect Models_. R package version 0.46-5.

A BibTeX entry for LaTeX users is

@Manual{,

```
title = {npmlreg: Nonparametric Maximum Likelihood Estimation for Random Effect
                                                                                                                                                                                                                                                                                                          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 0.46-5},
                                                                                                                                                                                                                                                                                                                                                                                            'help("citation")'.
                                                                                                                             year = \{2018\},\
                                             Models},
```

The correct citation for this R vignette is

42

EINBECK, J. and HINDE, J. (2014). Nonparametric maximum likelihood estimation for random effect models in R. Vignette to R package npmlreg.

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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 available in **npmlreg** is given below:

> ls("package:npmlreg")

"binomial.expand"	"expand.vc"	"tolfind"	
"allvc"	"expand"	"post"	.c.w"
"alldist"	"dkern"	"gqz"	"weightslogl.cal
님	4	5	10

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