

Nonparametric maximum likelihood estimation for random effect models in R

Vignette to R package **npmlreg**

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Contents

1	Introduction	3
2	Random effect modelling with exponential family mixtures	3
3	Examples	6
3.1	Finite Gaussian mixtures: The galaxy data	6
3.2	Compound Poisson models: The fabric faults data	20
3.3	Logistic regression with random effects: The toxoplasmosis data	24
3.4	Modelling mixtures of Gamma distributions: The hospital stay data	30
3.5	Variance component models: The Oxford school boys data	33
3.6	Spatial random effect models: Irish Suicide Data	41
4	Citation	41
5	References	42
6	Appendix: R Documentation	44

1 Introduction

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 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 `allvc` (for variance component 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

Assume there is given a set of explanatory vectors x_1, \dots, x_n and a set of observations y_1, \dots, y_n sampled from an exponential family 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 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`, Gaussian, 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

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

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

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

The score equations

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

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

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

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

$$\hat{\pi}_k = \frac{1}{n} \sum_i w_{ik} \quad (5)$$

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

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

or

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

In the special case of a normally distributed random effect, one can employ tabulated Gauss-Hermite integration points and their corresponding masses for z_k and π_k , respectively, and consider these values as constants (Hinde, 1982). Otherwise, they have to be calculated simultaneously during the EM algorithm as outlined above (one then usually takes the GH points/masses as starting points, which are scaled outwards ($tol > 1$) or inwards ($tol < 1$) by means of a scaling parameter tol). As in this case no parametric specification of the random effect distribution is necessary, one refers to this method as ‘Nonparametric Maximum Likelihood’ (NPMLE) 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

The data considered in this example are the recession velocities (in km/s) of 82 galaxies receding from our own, sampled from six well-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 **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 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)
> 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
> gal$v1000
[1] 9.172 9.350 9.483 9.558 9.775 10.227 10.406 16.084 16.170 18.419
[11] 18.552 18.600 18.927 19.052 19.070 19.330 19.343 19.349 19.440 19.473
[21] 19.529 19.541 19.547 19.663 19.846 19.856 19.863 19.914 19.918 19.973
[31] 19.989 20.166 20.175 20.179 20.196 20.215 20.221 20.415 20.629 20.795
[41] 20.821 20.846 20.875 20.986 21.137 21.137 21.492 21.701 21.814 21.921 21.960
[51] 22.185 22.209 22.242 22.249 22.314 22.374 22.495 22.746 22.747 22.888
[61] 22.914 23.206 23.241 23.263 23.484 23.538 23.542 23.666 23.706 23.711
[71] 24.129 24.285 24.289 24.366 24.717 24.990 25.633 26.960 26.995 32.065
[81] 32.789 34.279
```

and load the **npmllreg** package:

```

> 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

```

which is the same as a NPMLE 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))

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

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=gal1))
```

```

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.

```

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

Coefficients:

MASS1	MASS2
9.865	21.876

```

Component distribution - MLE of sigma:      3.026
Random effect distribution - standard deviation: 3.384072

```

Mixture proportions:

```

MASS1      MASS2
0.08694133 0.91305867
-2 log L:   461

> (galaxy.np3 <- alldist(v1000~1,random=~1,random.distribution='np',k=3,data=gal))

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

Call: alldist(formula = v1000 ~ 1, random = ~1, data = gal, k = 3,
               random.distribution = "np")

Coefficients:
MASS1  MASS2  MASS3
9.75   21.40  32.94

Component distribution - MLE of sigma: 2.079
Random effect distribution - standard deviation: 4.03618

Mixture proportions:
MASS1  MASS2  MASS3
0.08590000 0.87690389 0.03719611
-2 log L: 425.4

> (galaxy.np4 <- alldist(v1000~1,random=~1,random.distribution='np',k=4,data=gal))

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.

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

Coefficients:

	MASS1	MASS2	MASS3	MASS4
9.71	20.00	23.50	33.04	

Component distribution - MLE of sigma:

Random effect distribution - standard deviation:

1.315
4.345212

Mixture proportions:

	MASS1	MASS2	MASS3	MASS4
0.08536797	0.52624187	0.35180277	0.03658738	

-2 log L:
416.5

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).

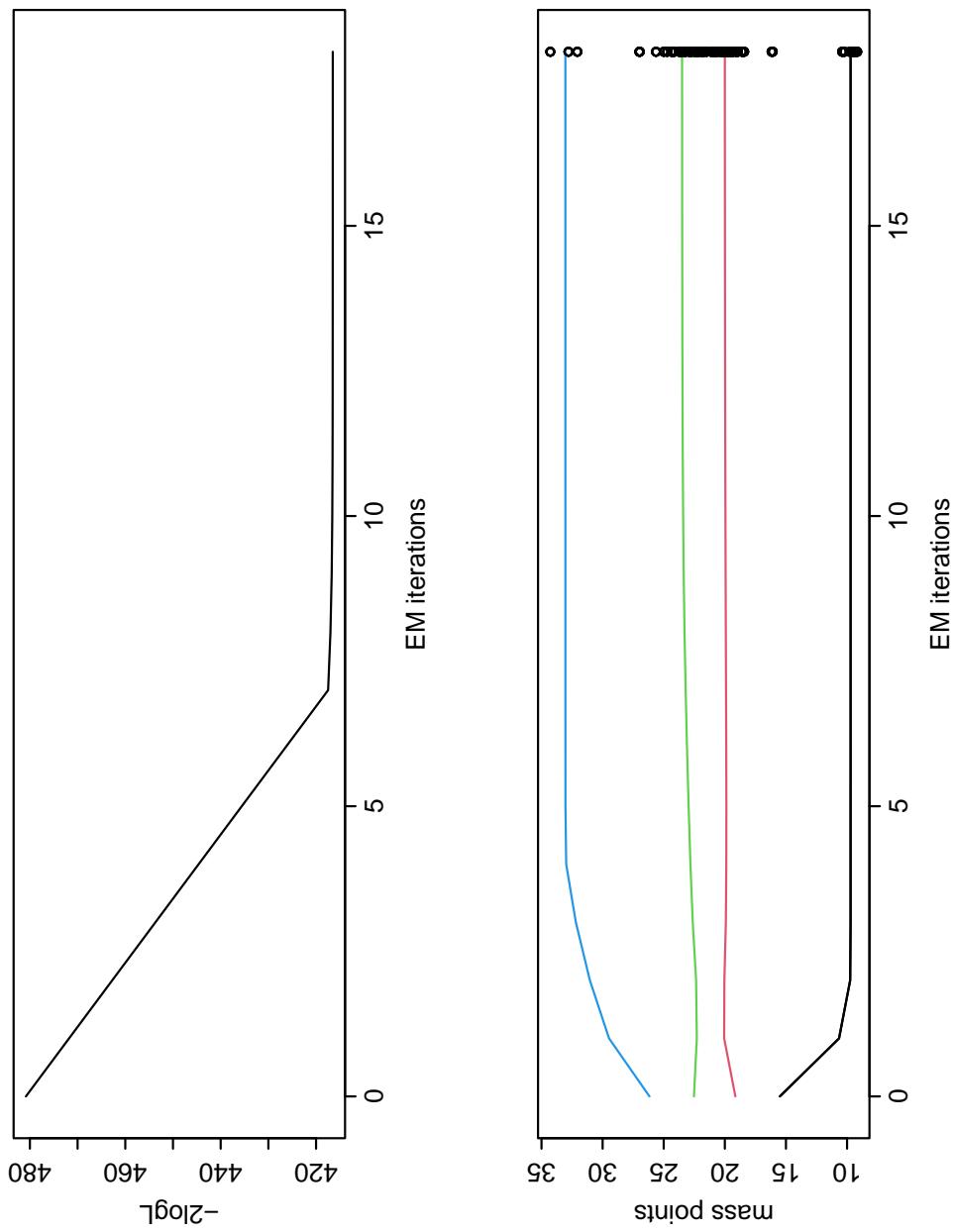


Fig. 1: Convergence of EM algorithm for NPMML estimation with 4 mass points. Top: Disparities; Bottom: EM Trajectories.

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))$disp
[1] 410.6852
> (galaxy.np6 <- alldist(v1000~1,random=~1,k=6,to1=0.2,data=gal, verbose=FALSE))$disp
[1] 394.5811
> (galaxy.np7 <- alldist(v1000~1,random=~1,k=7,to1=0.12,data=gal, verbose=FALSE))$disp
[1] 388.8639
> (galaxy.np8 <- alldist(v1000~1,random=~1,k=8,to1=0.2,data=gal, verbose=FALSE))$disp
[1] 388.1177
> (galaxy.np9 <- alldist(v1000~1,random=~1,k=9,to1=0.06,data=gal, verbose=FALSE))$disp
[1] 388.2149
```

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 < 1` 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 is 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 , $k = 1, \dots, K$ varying over the components, the possibility of smoothing the standard deviations among components is implemented. Smoothing is performed by means of the discrete kernel

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

(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))

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

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	1.68666727	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 ($y_i - x_i \hat{\beta}$), respectively. In the former plot (Fig. 2 left bottom), one sees nicely how the predicted values are ‘flattened’ within the clusters 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.

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 in a somewhat makeshift manner using the *equal* dispersion parameter for the ϕ preceding the log-likelihood, and the *unequal* dispersion parameters within the log-likelihood. Hence, it is strictly recommended to work with the deviance rather than with the disparity in the case of unequal component dispersion parameters, as 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.

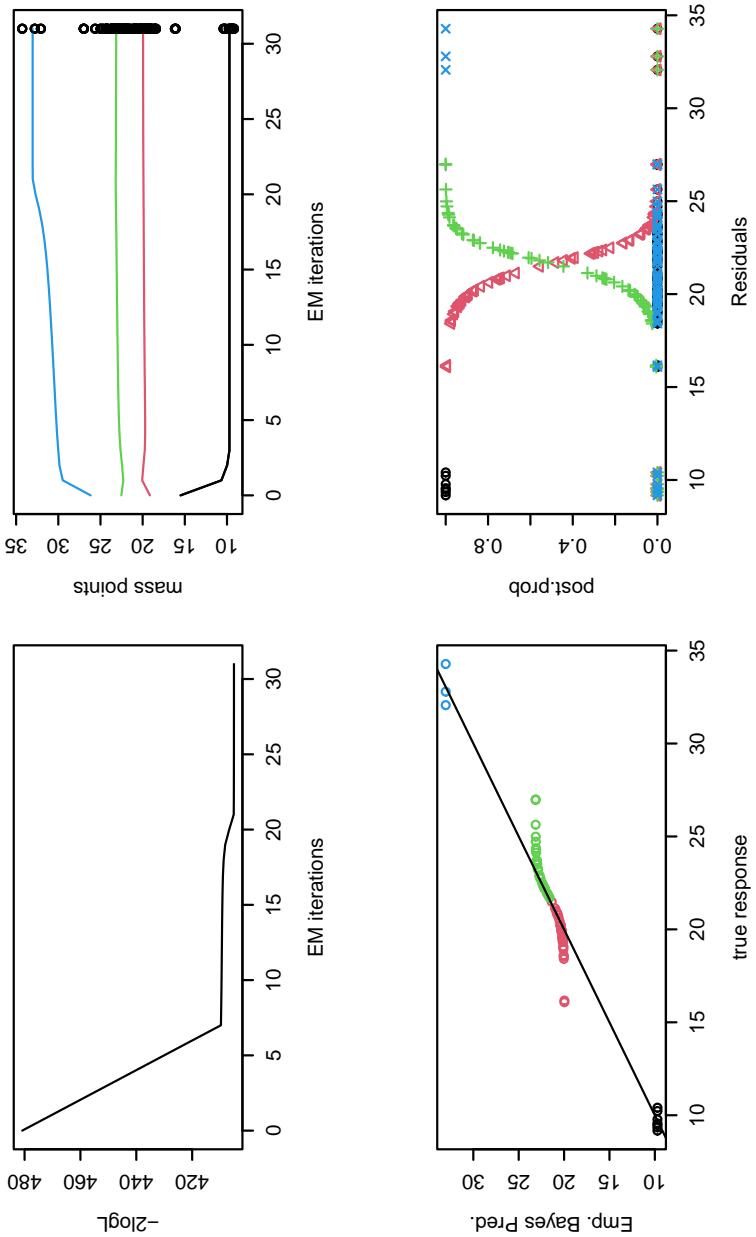


Fig. 2: Diagnostic plots for NPMIL estimation with unequal variances and 4 mass points. One might fear that for a high number of mass points some component standard deviations could tend to zero. This can indeed be

the case. Using 8 instead of 4 mass points in the call above one gets the error message

```
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.
```

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 than 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. For instance, running

```
> (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
```

```
[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
```

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:

```
> (galaxy.np8ud <- alldist(v1000~1, random=~1, k=8, tol=0.5, data=gal1, 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
EM algorithm met convergence criteria at iteration # 102
Disparity trend plotted.
EM Trajectories plotted.
```

Call: alldist(formula = v1000 ~ 1, random = ~1, data = gal1, 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	MASS6	MASS7	MASS8
7.888540e-15	8.536585e-02	2.439018e-02	4.039238e-01	4.256102e-01				
2.412464e-02	2.439092e-02	1.219444e-02						
-2 log L:	374.6							

```
> galaxy.np8ud$sddev$sddev
[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.

```

> 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

Minimal Disparity: 219.9949 at tol= 0.5
Minimal Disparity with EM converged: 357.8216 at tol= 0.4
$AllDisparities
[1] 1233.6883 387.2360 377.6917 377.0345 360.9393 359.4521 357.8221
[8] 357.8216 323.3126 219.9949 363.8772 Inf

$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

```

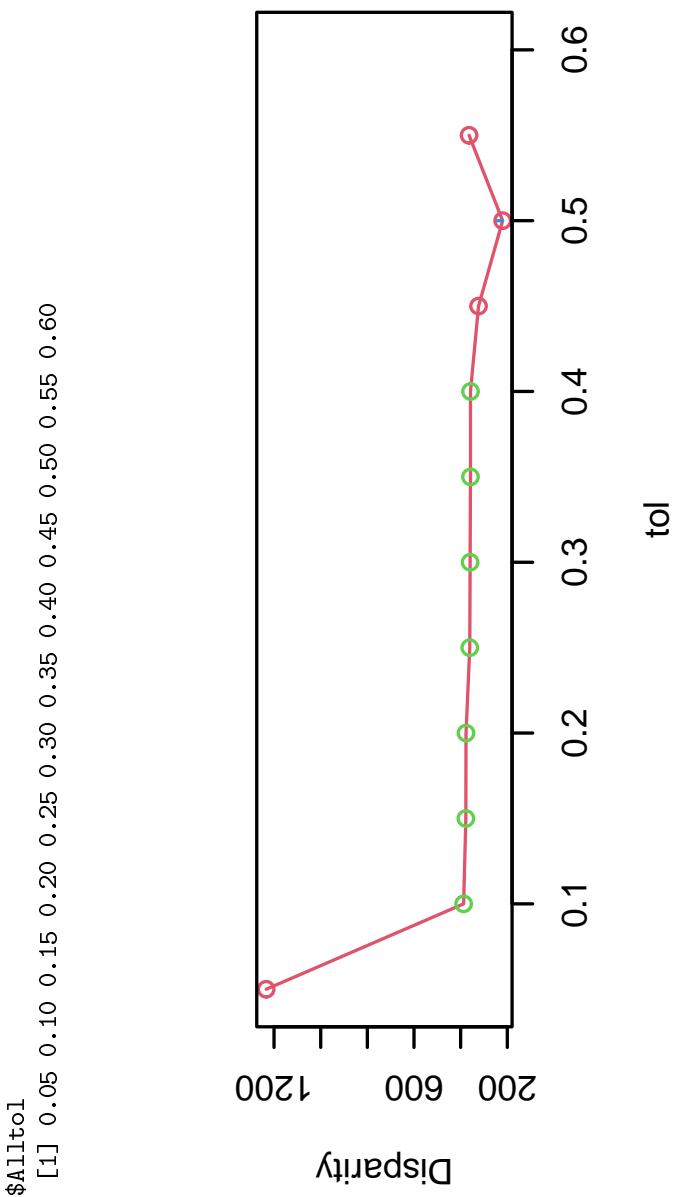


Fig. 3: Disparity against tol for 8 mass point model with unequal variances. Green circles: EM converged; red circles: EM not converged.

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)
> (faults0 <- glm(y ~ 1, family=poisson(link=log), data=fabric))
Call: glm(formula = y ~ 1, family = poisson(link = log), data = fabric)

Coefficients:
(Intercept) 2.183

Degrees of Freedom: 31 Total (i.e. Null); 31 Residual
Null Deviance: 103.7 AIC: 229
Residual Deviance: 103.7 AIC: 229

> (faults1 <- glm(y ~ x, family=poisson(link=log), data=fabric))
Call: glm(formula = y ~ x, family = poisson(link = log), data = fabric)

Coefficients:
(Intercept) x
-4.1730    0.9969

Degrees of Freedom: 31 Total (i.e. Null); 30 Residual
Null Deviance: 103.7 AIC: 191.8
Residual Deviance: 64.54 AIC: 191.8
```

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 basic 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.

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

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

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"))

1 ..2 ..3 ..4 ..5 ..6 ..
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")
```

```

Coefficients:
(Intercept)          x          z
-4.4128           1.0331    0.3391
Random effect distribution - standard deviation: 0.3391081

-2 log L:          175.6

> (faults.g3<- alldist(y ~ x, family=poisson(link=log), random=~1, data= fabric, k=3, random.distribution="gq", verbose=F))

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

```

```

Coefficients:
(Intercept)          x          z
-3.3089           0.8488    0.3575
Random effect distribution - standard deviation: 0.3574909

-2 log L:          174.3

```

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

```

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 NPMI:

```

> (faults.np2<- alldist(y ~ x, family=poisson(link=log), random=~1, 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 ..
EM algorithm met convergence criteria at iteration # 22
Disparity trend plotted.
EM Trajectories plotted.

```

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

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

```
> (faults.np3<- alldist(y ~ x, family=poisson(link=log), random=~1, data=fabric,k=3, random.distribution="np", verbose=FALSE))
```

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

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 0.66666708 0.2014057
-2 log L:   172.7

```

The disparities are not far from those obtained with Gaussian quadrature, indicating that the random effect distribution is not very far from a normal distribution. While three mass points seem to be adequate for GQ, only two mass points are needed with NPMML. Note 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

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 analytical mean of the marginal distribution, considering `faults[1:6,]` as ‘new’ input data (Aitkin, Hinde & Francis, 2005, p. 459), and in the second case in an empirical Bayes approach (Aitkin, 1996a) using the individual posterior probabilities obtained as a by-product 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 NPMI. 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)))
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) ~ 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	0.57062599	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.npx$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)))
```

```
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:

MASS1	MASS2	MASS3
0.33215441	0.57878769	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.npxx<- alldist(cbind(Cases,Total-Cases)~x, random=~x, 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 # 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
                                         0.8089833

Random effect distribution - standard deviation:
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  $w_{ik}$ 
> round(t(toxo.np$post.prob), digits=2)

```

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
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
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

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 posterior 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:

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

卷之三

```
> 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
34
0.5638

```

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

```

> predict(toxo.np, type="response")
    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 0.5382 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

or, even quicker,
> fitted(toxo.np)
    1     2     3     4     5     6     7     8
0.4802916 0.3621653 0.3646799 0.3621653 0.5363293 0.5161203 0.3493630 0.3893228
    9    10    11    12    13    14    15    16
0.4898596 0.5881705 0.2920528 0.4193273 0.5350387 0.2747238 0.4193273 0.5283871
    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 0.5533823 0.3621653
    33    34
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)
> (fitnp3<- alldist(duration~age+temp1, data=hosp, k=3, family=Gamma(link=log), tol=0.2))
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 ..
EM algorithm met convergence criteria at iteration # 27
Disparity trend plotted.
EM Trajectories plotted.
```

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

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 0.11220988  
-2 log L: 121.3
```

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 listed 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), tol=0.2, shape=1))  
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 # 41  
Disparity trend plotted.  
EM Trajectories plotted.
```

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

Coefficients:

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

Component distribution - MLE of shape parameter:
Random effect distribution - standard deviation:

1
3.118363e-15

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).

One important remark should still be given. When employing the damped EM algorithm, one will very occasionally observe rising disparities, typically from about the 10th to the 30th EM iteration. According to the theory on EM, this shouldn't happen. This 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 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. This can be achieved by setting the constant `damp.power` in the formula

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

to a value bigger than one, where `iter` 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

```

> data(Oxboys, package = "nlme")
> Oxboys$boy <- g1(26, 9)
> plot(Oxboys$age[Oxboys$boy==1], Oxboys$height[Oxboys$boy==1], ylim=c(125, 175), type='b', pch=1, xlab='age', ylab='height')
> for (i in 2:nlevels(Oxboys$Subject)) {lines(Oxboys$age[Oxboys$Subject==i], Oxboys$height[Oxboys$boy==i], lty=1, type='b', col=i)}

```

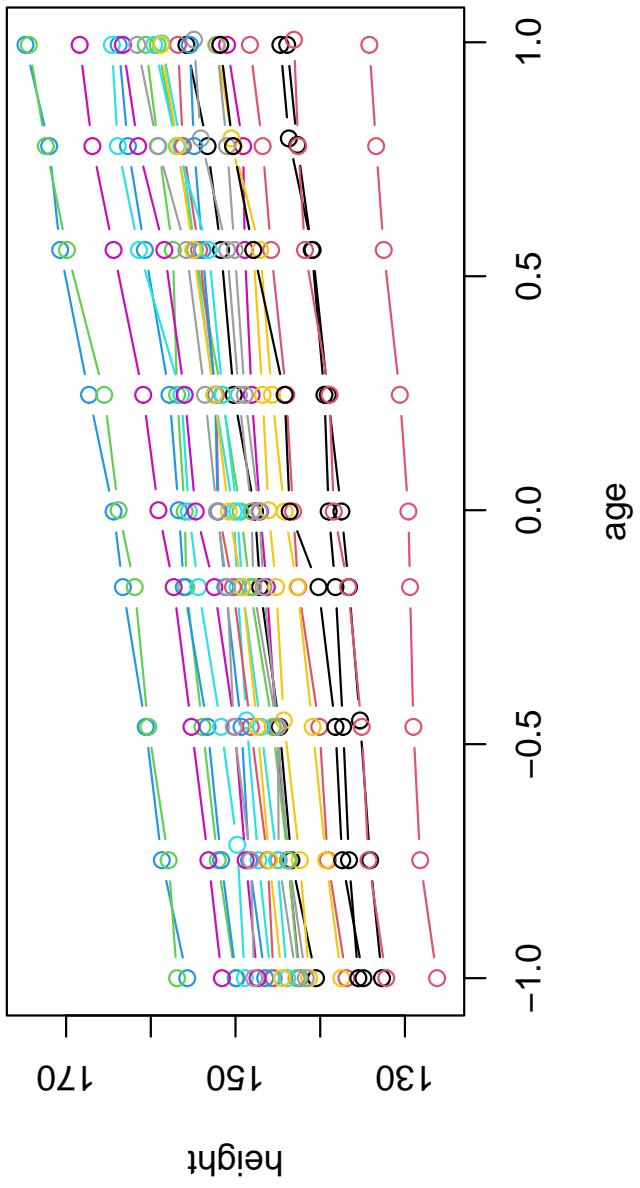


Fig. 4: Oxford Boys Data

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), one gets

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

Call: allvc(formula = height ~ age, random = ~1 | boy, data = Oxbboys,
            k = 20, random.distribution = "gq")

Coefficients:
(Intercept)      age          z
148.958        6.524       4.769

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

-2 log L: 991.8
```

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 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 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

```
> Oxbboys.g20$rsdev^2 / (Oxbboys.g20$rsdev^2 + Oxbboys.g20$sderv^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 NPMI estimation. For illustration, we fit NPMI with seven (as suggested by Aitkin, Hinde & Francis (2005), p. 495), and eight masspoints, yielding

```
> (0xboys.np7 <- allvc(height~age,random=~1/boy,data=0xboys,random.distribution='np',k=7))
```

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

```
Call: allvc(formula = height ~ age, random = ~1 | boy, data = 0xboys,
           k = 7, random.distribution = "np")
```

Coefficients:

age	MASS1	MASS2	MASS3	MASS4	MASS5	MASS6	MASS7
6.524	130.200	138.417	144.605	149.967	155.261	159.521	164.884

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

Mixture proportions:

MASS1	MASS2	MASS3	MASS4	MASS5	MASS6	MASS7
0.03846154	0.11538462	0.19303307	0.34544795	0.19228146	0.03846828	
0.07692308						
-2 log L:						1017.3

```
> (0xboys.np8 <- allvc(height~age,random=~1/boy,data=0xboys,random.distribution='np',k=8))
```

```

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

```

```
Call: allvc(formula = height ~ age, random = ~1 | boy, data = Oxboys,
           k = 8, random.distribution = "np")
```

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							
164.884							

Component distribution - MLE of sigma:

Random effect distribution - standard deviation:

1.433

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, NPMIL 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)
```

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

```
> (0xboys.np8s <- allvc(height~age,random=~age/boy,data=0xboys,random.distribution='np',k=8))
```

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

EM algorithm met convergence criteria at iteration # 10

Disparity trend plotted.

EM Trajectories plotted.

```
Call: allvc(formula = height ~ age, random = ~age | boy, data = 0xboys, k = 8, random.distribution = "np")
```

Coefficients:

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

Component distribution - MLE of sigma: 1.185

Random effect distribution - standard deviation: 7.893352

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					
-2 log L:		842.4				

The difference in disparities is

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

[1] 88.93035

on 7df, showing clear heterogeneity in the slope.

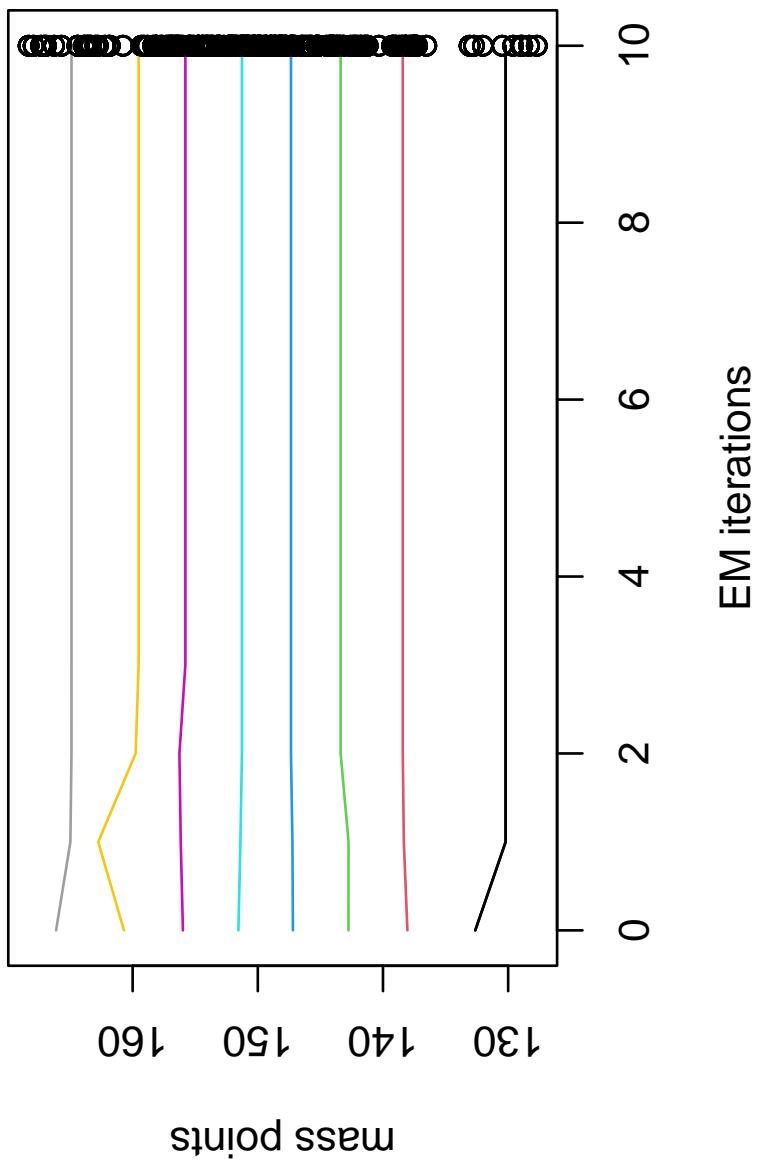


Fig. 5: Convergence of EM for eight mass points, applied on Oxford boys data.

3.6 Spatial random effect models: Irish Suicide Data

The data considered here, available in the package `npmlreg` via

```
> data(irlsuicide)
```

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 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 effect accounts for within-region correlation, it is worthwhile 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 and Hinde (2006).

4 Citation

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, <<https://CRAN.R-project.org/package=npmlreg>>.

A BibTeX entry for LaTeX users is

```
@Manual{,
```

```

title = {npmlreg: Nonparametric Maximum Likelihood Estimation for Random Effect
Models},
author = {Jochen Einbeck and Ross Darnell and John Hinde},
year = {2018},
note = {R package version 0.46-5},
url = {https://CRAN.R-project.org/package=npmlreg},
}

```

ATTENTION: This citation information has been auto-generated from the package DESCRIPTION file and may need manual editing, see `help("citation")`.

The correct citation for this R vignette is

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

Acknowledgments

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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")  
[1] "alldist"          "allvc"  
[4] "dkern"            "expand"  
[7] "gqz"              "post"  
[10] "weightslog1.calc.w"
```

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