

# Package ‘mixAK’

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**Title** Multivariate Normal Mixture Models and Mixtures of Generalized Linear Mixed Models Including Model Based Clustering

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**Depends** R (>= 3.0.0), colorspace, lme4 (>= 1.0)

**Imports** graphics, stats, splines, fastGHQuad, mnormt, parallel, coda

**Description** Contains a mixture of statistical methods including the MCMC methods to analyze normal mixtures. Additionally, model based clustering methods are implemented to perform classification based on (multivariate) longitudinal (or otherwise correlated) data. The basis for such clustering is a mixture of multivariate generalized linear mixed models.

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Acidity	<i>Acidity index of lakes in North-Central Wisconsin</i>
---------	--

---

### Description

Acidity index measured in a sample of 155 lakes in North-Central Wisconsin.

Crawford et al. (1992) and Crawford (1994) analyzed these data as a mixture of normal distributions on the log-scale. Richardson and Green (1997) used a normal mixture estimated using reversible jump MCMC.

### Usage

```
data(Acidity)
```

### Format

A numeric vector with observed values.

### Source

<http://www.stats.bris.ac.uk/~peter/mixdata>

### References

Crawford, S. L. (1994). An application of the Laplace method to finite mixture distribution. *Journal of the American Statistical Association*, **89**, 259–267.

Crawford, S. L., DeGroot, M. H., Kadane, J. B., and Small, M. J. (1994). Modeling lake chemistry distributions: Approximate Bayesian methods for estimating a finite mixture model. *Technometrics*, **34**, 441–453.

Richardson, S. and Green, P. J. (1997). On Bayesian analysis of mixtures with unknown number of components (with Discussion). *Journal of the Royal Statistical Society, Series B*, **59**, 731–792.

### Examples

```
data(Acidity)
summary(Acidity)
```

---

autolayout	<i>Automatic layout for several plots in one figure</i>
------------	---

---

**Description**

Returns a matrix which can be used in [layout](#) function as its mat argument.

**Usage**

```
autolayout(np)
```

**Arguments**

np                    number of plots that are to be produced on 1 figure

**Value**

A matrix.

**Author(s)**

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

**See Also**

[par.](#)

**Examples**

```
autolayout(10)
```

---

BLA	<i>Best linear approximation with respect to the mean square error (theoretical linear regression).</i>
-----	---

---

**Description**

For a random vector  $\mathbf{X} = (X_1, \dots, X_p)'$  for which a mean and a covariance matrix are given computes coefficients of the best linear approximations with respect to the mean square error of each component of  $\mathbf{X}$  given the remaining components of  $\mathbf{X}$ .

**Usage**

```
BLA(mean=c(0, 0), Sigma=diag(2))
```

**Arguments**

mean            a numeric vector of means.  
 Sigma           a covariance matrix.

**Value**

A list with the following components:

beta            computed regression coefficients  
 sigmaR2        residual variances

**Author(s)**

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

**References**

Anděl, J. (2007, odd. 2.5). *Základy matematické statistiky*. Praha: MATFYZPRESS.

**Examples**

```
##### X = (U(1), U(2), U(3))'
##### * U(1) <= U(2) <= U(3)
##### * ordered uniform Unif(0, 1) variates
EX <- (1:3)/4
varX <- matrix(c(3,2,1, 2,4,2, 1,2,3), ncol=3)/80
BLA(EX, Sigma=varX)

##### Uroda sena
##### * Y1 = uroda sena [cent/akr]
##### * Y2 = jarni srazky [palce]
##### * Y3 = kumulovana teplota nad 42 F
EY <- c(28.02, 4.91, 28.7)
varY <- matrix(c(19.54, 3.89, -3.76, 3.89, 1.21, -1.31, -3.76, -1.31, 4.52), ncol=3)
BLA(EY, Sigma=varY)

##### Z=(X, Y) ~ uniform distribution on a triangle
##### M = {(x,y): x>=0, y>=0, x+y<=3}
EZ <- c(1, 1)
varZ <- matrix(c(2, -1, -1, 2), nrow=2)/4
BLA(EZ, Sigma=varZ)

##### W=(X, Y) ~ uniform distribution on
##### M = {(x,y): x>=0, 0<=y<=1, y<=x<=y+1}
EW <- c(1, 1/2)
varW <- matrix(c(2, 1, 1, 1), nrow=2)/12
BLA(EW, Sigma=varW)
```

BsBasis

*B-spline basis***Description**

It creates a B-spline basis based on a specific dataset. B-splines are assumed to have common boundary knots and equidistant inner knots.

**Usage**

```
BsBasis(degree, ninner, knotsBound, knots, intercept=FALSE,
        x, tgrid, Bname="B", plot=FALSE, lwd=1,
        col="blue", xlab="Time", ylab="B(t)",
        pch=16, cex.pch=1, knotcol="red")
```

**Arguments**

degree	degree of the B-spline.
ninner	number of inner knots.
knotsBound	2-component vector with boundary knots.
knots	knots of the B-spline (including boundary ones). If knots is given ninner and knotsBound are ignored.
intercept	logical, if FALSE, the first basis B-spline is removed from the B-spline basis and it is assumed that intercept is added to the statistical models used afterwards.
x	a numeric vector to be used to create the B-spline basis.
tgrid	if given then it is used to plot the basis.
Bname	label for the created columns with the B-spline basis.
plot	logical, if TRUE the B-spline basis is plotted.
lwd, col, xlab, ylab	arguments passed to the plotting function.
pch, cex.pch	plotting character and cex used to plot knots
knotcol	color for knots on the plot with the B-spline basis.

**Value**

A matrix with the B-spline basis. Number of rows is equal to the length of x.

Additionally, the resulting matrix has attributes:

degree	B-spline degree
intercept	logical indicating the presence of the intercept B-spline
knots	a numeric vector of knots
knotsInner	a numeric vector of inner knots
knotsBound	a numeric vector of boundary knots

df	the length of the B-spline basis (number of columns of the resulting object).
tgrid	a numeric vector which can be used on x-axis to plot the basis.
Xgrid	a matrix with length(tgrid) rows and df columns which can be used to plot the basis.

**Author(s)**

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

**See Also**

[bs](#).

**Examples**

```
set.seed(20101126)
t <- runif(20, 0, 100)

oldPar <- par(mfrow=c(1, 2), bty="n")
Bs <- BsBasis(degree=3, ninner=3, knotsBound=c(0, 100), intercept=FALSE,
              x=t, tgrid=0:100, plot=TRUE)
print(Bs)

Bs2 <- BsBasis(degree=3, ninner=3, knotsBound=c(0, 100), intercept=TRUE,
               x=t, tgrid=0:100, plot=TRUE)
print(Bs2)
par(oldPar)

print(Bs)
print(Bs2)
```

---

cbplot

*Plot a function together with its confidence/credible bands*

---

**Description**

This routine typically plots a function together with its confidence or credible bands. The credible band can be indicated either by additional lines or by a shaded region or by both.

**Usage**

```
cbplot(x, y, low, upp, type=c("l", "s"), band.type=c("ls", "s", "l"), add=FALSE,
        col="darkblue", lty=1, lwd=2,
        cbc=col, cblty=4, cblwd=lwd,
        scol=rainbow_hcl(1, start=180, end=180), slwd=5,
        xlim, ylim, xlab, ylab, main="", sub="", cex.lab=1, cex.axis=1, ...)
```

**Arguments**

x	a numeric vector with x coordinates corresponding to y, low, upp.
y	a numeric vector with y coordinates of the function to plot.
low	a numeric vector with y coordinates of the lower limit of the credible band.
upp	a numeric vector with y coordinates of the upper limit of the credible band.
type	argument with the same meaning as type in <code>plot.default</code> .
band.type	a character which specifies the graphical way to show the credible band, “ls” stands for line and shaded region, “s” stands for shaded region only and “l” stands for line only.
add	if TRUE then everything is added to the current plot.
col, lty, lwd	graphical parameters to draw the x-y line.
cbcol, cblty, cblwd	graphical parameters to draw the x-low and x-upp lines.
scol, slwd	graphical parameters for the shaded region between the credible/confidence bounds.
xlim, ylim, xlab, ylab, main, sub, cex.lab, cex.axis	other graphical parameters.
...	additional arguments passed to the plot function.

**Value**

`invisible(x)`

**Author(s)**

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

**Examples**

```
### Artificial credible bands around the CDF's of N(100, 15*15)
### and N(80, 10*10)
iq <- seq(55, 145, length=100)
Fiq <- pnorm(iq, 100, 15)
low <- Fiq - 0.1
upp <- Fiq + 0.1

iq2 <- seq(35, 125, length=100)
Fiq2 <- pnorm(iq, 80, 10)
low2 <- Fiq2 - 0.1
upp2 <- Fiq2 + 0.1

cbplot(iq, Fiq, low, upp, xlim=c(35, 145))
cbplot(iq2, Fiq2, low2, upp2, add=TRUE, col="red4",
       scol=rainbow_hcl(1, start=20, end=20))
```



---

Dirichlet

*Dirichlet distribution*

---

### Description

Random number generation for the Dirichlet distribution  $D(\alpha_1, \dots, \alpha_K)$ .

### Usage

```
rDirichlet(n, alpha=c(1, 1))
```

### Arguments

n	number of observations to be sampled.
alpha	parameters of the Dirichlet distribution ('prior sample sizes').

### Value

Some objects.

### Value for rDirichlet

A matrix with sampled values.

### Author(s)

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

### References

- Devroye, L. (1986). *Non-Uniform Random Variate Generation*. New York: Springer-Verlag, Chap. XI.
- Gelman, A., Carlin, J. B., Stern, H. S., and Rubin, D. B. (2004). *Bayesian Data Analysis. Second Edition*. Boca Raton: Chapman and Hall/CRC, pp. 576, 582.

### See Also

[rbeta](#).

### Examples

```
set.seed(1977)

alpha <- c(1, 2, 3)
Mean <- alpha/sum(alpha)
Var <- -(alpha %*% t(alpha))
diag(Var) <- diag(Var) + alpha*sum(alpha)
Var <- Var/(sum(alpha)^2*(1+sum(alpha)))
```

```
x <- rDirichlet(1000, alpha=alpha)
x[1:5,]

apply(x, 1, sum)[1:5]          ### should be all ones
rbind(Mean, apply(x, 2, mean))

var(x)
print(Var)
```

---

Enzyme

*Enzymatic activity in the blood*

---

### Description

Enzymatic activity in the blood, for an enzyme involved in the metabolism of carcinogenic substances, among a group of 245 unrelated individuals.

Bechtel et al. (1993) identified a mixture of two skewed distributions by using maximum-likelihood estimation. Richardson and Green (1997) used a normal mixture estimated using reversible jump MCMC to estimate the distribution of the enzymatic activity.

### Usage

```
data(Enzyme)
```

### Format

A numeric vector with observed values.

### Source

<http://www.stats.bris.ac.uk/~peter/mixdata>

### References

Bechtel, Y. C., Bonaïti-Pellié, C., Poisson, N., Magnette, J., and Bechtel, P. R. (1993). A population and family study of N-acetyltransferase using caffeine urinary metabolites. *Clinical Pharmacology and Therapeutics*, **54**, 134–141.

Richardson, S. and Green, P. J. (1997). On Bayesian analysis of mixtures with unknown number of components (with Discussion). *Journal of the Royal Statistical Society, Series B*, **59**, 731–792.

### Examples

```
data(Enzyme)
summary(Enzyme)
```

---

Faithful

*Old Faithful Geysers Data*

---

### Description

Waiting time between eruptions and the duration of the eruption for the Old Faithful geyser in Yellowstone National Park, Wyoming, USA, version used in Härdle, W. (1991).

### Usage

```
data(Faithful)
```

### Format

A data frame with 272 observations on 2 variables.

eruptions eruption time in minutes

waiting waiting time to the next eruption in minutes

### Details

There are many versions of this dataset around. Azzalini and Bowman (1990) use a more complete version.

### Source

R package MASS

### References

Härdle, W. (1991). *Smoothing Techniques with Implementation in S*. New York: Springer.

Azzalini, A. and Bowman, A. W. (1990). A look at some data on the Old Faithful geyser. *Applied Statistics*, **39**, 357-365.

### See Also

[geyser](#).

### Examples

```
data(Faithful)
summary(Faithful)
```

---

fitted.GLMM\_MCMC      *Fitted profiles in the GLMM model*

---

### Description

It calculates fitted profiles in the (multivariate) GLMM with a normal mixture in the random effects distribution based on selected posterior summary statistic of the model parameters.

### Usage

```
## S3 method for class 'GLMM_MCMC'
fitted(object, x, z,
        statistic=c("median", "mean", "Q1", "Q3", "2.5%", "97.5%"),
        overall=FALSE, glmer=TRUE, nAGQ=100, ...)
```

### Arguments

object	object of class <a href="#">GLMM_MCMC</a> .
x	matrix or list of matrices (in the case of multiple responses) for “fixed effects” part of the model used in the calculation of fitted values.
z	matrix or list of matrices (in the case of multiple responses) for “random effects” part of the model used in the calculation of fitted values.
statistic	character which specifies the posterior summary statistic to be used to calculate fitted profiles. Default is the posterior median. It applies only to the overall fit.
overall	logical. If TRUE, fitted profiles based on posterior mean/median/Q1/Q3/2.5%/97.5% of the model parameters are computed. If FALSE, fitted profiles based on posterior means given mixture component are calculated. Note that this depends on used re-labelling of the mixture components and hence might be misleading if re-labelling is not succesfull!
glmer	a logical value. If TRUE, the real marginal means are calculated using Gaussian quadrature.
nAGQ	number of quadrature points used when glmer is TRUE.
...	possibly extra arguments. Nothing useful at this moment.

### Value

A list (one component for each of multivariate responses from the model) with fitted values calculated using the x and z matrices. If overall is FALSE, these are then matrices with one column for each mixture component.

### Author(s)

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

**See Also**

[GLMM\\_MCMC](#).

**Examples**

```
### WILL BE ADDED.
```

---

Galaxy

*Velocities of distant galaxies*

---

**Description**

Velocities (in km/sec) of 82 distant galaxies, diverging from our own galaxy.

The dataset was first described by Roeder (1990) and subsequently analysed under different mixture models by several researchers including Escobar and West (1995) and Phillips and Smith (1996). Richardson and Green (1997) used a normal mixture estimated using reversible jump MCMC to estimate the distribution of the velocities.

**REMARK:** 78th observation is here 26.96 whereas it should be 26.69 (see [galaxies](#)). A value of 26.96 used in Richardson and Green (1997) is kept here.

**Usage**

```
data(Galaxy)
```

**Format**

A numeric vector with observed values.

**Source**

<http://www.stats.bris.ac.uk/~peter/mixdata>

**References**

Escobar, M. D. and West, M. (1995). Bayesian density estimation and inference using mixtures. *Journal of the American Statistical Association*, **90**, 577–588.

Phillips, D. B. and Smith, A. F. M. (1996). Bayesian model comparison via jump diffusions. In *Practical Markov Chain Monte Carlo*, eds: W. R. Gilks, S. Richardson, and D. J. Spiegelhalter, ch. 13, pp. 215-239. London: Chapman and Hall.

Richardson, S. and Green, P. J. (1997). On Bayesian analysis of mixtures with unknown number of components (with Discussion). *Journal of the Royal Statistical Society, Series B*, **59**, 731–792.

Roeder, K. (1990). Density estimation with confidence sets exemplified by superclusters and voids in the galaxies. *Journal of the American Statistical Association*, **85**, 617–624.

**See Also**

[galaxies](#).

**Examples**

```
data(Galaxy)
summary(Galaxy)
```

---

generatePermutations *Generate all permutations of (1, ..., K)*

---

**Description**

It generates a matrix containing all permutations of (1, ..., K).

**Usage**

```
generatePermutations(K)
```

**Arguments**

K                    integer value of  $K$ .

**Value**

A matrix of dimension  $K! \times K$  with generated permutations in rows.

**Author(s)**

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

**Examples**

```
generatePermutations(1)
generatePermutations(2)
generatePermutations(3)
generatePermutations(4)
```

---

getProfiles	<i>Individual longitudinal profiles of a given variable</i>
-------------	---

---

### Description

It creates a list with individual longitudinal profiles of a given variable.

### Usage

```
getProfiles(t, y, id, data)
```

### Arguments

t	a character string giving the name of the variable with “time”.
y	a character string giving the names of the responses variables to keep in the resulting object.
id	a character string giving the name of the variable which identifies subjects.
data	a data.frame with all the variables.

### Value

A list of data.frames, one for each subject identified by id in the original data.

### Author(s)

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

### See Also

[plotProfiles](#).

### Examples

```
data(PBCseq, package="mixAK")
ip <- getProfiles(t="day", y=c("age", "lbili", "platelet", "spiders"),
                 id="id", data=PBCseq)
print(ip[[2]])
print(ip[[34]])

XLIM <- c(0, 910)
lcol1 <- rainbow_hcl(1, start=40, end=40)

oldPar <- par(mfrow=c(1, 3), bty="n")
plotProfiles(ip=ip, data=PBCseq, xlim=XLIM, var="lbili", tvar="day",
             xlab="Time (days)", col=lcol1, auto.layout=FALSE, main="Log(bilirubin)")
plotProfiles(ip=ip, data=PBCseq, xlim=XLIM, var="platelet", tvar="day",
             xlab="Time (days)", col=lcol1, auto.layout=FALSE, main="Platelet count")
plotProfiles(ip=ip, data=PBCseq, xlim=XLIM, var="spiders", tvar="day",
```

```

      xlab="Time (days)", col=1col1, auto.layout=FALSE)
par(oldPar)

```

---

GLMM_longitDA	<i>Discriminant analysis for longitudinal profiles based on fitted GLMM's</i>
---------------	---

---

### Description

The idea is that we fit (possibly different) GLMM's for data in training groups using the function [GLMM\\_MCMC](#) and then use the fitted models for discrimination of new observations. For more details we refer to Komárek et al. (2010).

Currently, only continuous responses for which linear mixed models are assumed are allowed.

### Usage

```
GLMM_longitDA(mod, w.prior, y, id, time, x, z, xz.common=TRUE, info)
```

### Arguments

mod	a list containing models fitted with the <a href="#">GLMM_MCMC</a> function. Each component of the list is the GLMM fitted in the training dataset of each cluster.
w.prior	a vector with prior cluster weights. The length of this argument must be the same as the length of argument mod. Can also be given relatively, e.g., as <code>c(1, 1)</code> which means that both prior weights are equal to 1/2.
y	vector, matrix or data frame (see argument y of <a href="#">GLMM_MCMC</a> function) with responses of objects that are to be clustered.
id	vector which determines clustered observations (see also argument y of <a href="#">GLMM_MCMC</a> function).
time	vector which gives indices of observations within clusters. It appears (together with id) in the output as identifier of observations
x	see <code>xz.common</code> below.
z	see <code>xz.common</code> below.
xz.common	a logical value. If TRUE then it is assumed that the X and Z matrices are the same for GLMM in each cluster. In that case, arguments x and z have the same structure as arguments x and z of <a href="#">GLMM_MCMC</a> function. If FALSE then X and Z matrices for the GLMM may differ across clusters. In that case, arguments x and z are both lists of length equal to the number of clusters and each component of lists x and z has the same structure as arguments x and z of <a href="#">GLMM_MCMC</a> function.
info	interval in which the function prints the progress of computation



**Details**

This function complements a paper Komárek et al. (2010).

**Value**

A list with the following components:

ident	ADD DESCRIPTION
marg	ADD DESCRIPTION
cond	ADD DESCRIPTION
ranef	ADD DESCRIPTION

**Author(s)**

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

**References**

Komárek, A., Hansen, B. E., Kuiper, E. M. M., van Buuren, H. R., and Lesaffre, E. (2010). Discriminant analysis using a multivariate linear mixed model with a normal mixture in the random effects distribution. *Statistics in Medicine*, **29**(30), 3267–3283.

**See Also**

[GLMM\\_MCMC](#), [GLMM\\_longitDA2](#).

**Examples**

```
### WILL BE ADDED.
```

---

GLMM_longitDA2	<i>Discriminant analysis for longitudinal profiles based on fitted GLMM's</i>
----------------	---

---

**Description**

WILL BE ADDED.

**Usage**

```
GLMM_longitDA2(mod, w.prior, y, id, x, z, xz.common = TRUE,  
               keep.comp.prob = FALSE, level = 0.95,  
               info, silent = FALSE)
```

**Arguments**

<code>mod</code>	a list containing models fitted with the <a href="#">GLMM_MCMC</a> function. Each component of the list is the GLMM fitted in the training dataset of each cluster.
<code>w.prior</code>	a vector with prior cluster weights. The length of this argument must be the same as the length of argument <code>mod</code> . Can also be given relatively, e.g., as <code>c(1, 1)</code> which means that both prior weights are equal to 1/2.
<code>y</code>	vector, matrix or data frame (see argument <code>y</code> of <a href="#">GLMM_MCMC</a> function) with responses of objects that are to be clustered.
<code>id</code>	vector which determines clustered observations (see also argument <code>y</code> of <a href="#">GLMM_MCMC</a> function).
<code>x</code>	see <code>xz.common</code> below.
<code>z</code>	see <code>xz.common</code> below.
<code>xz.common</code>	a logical value. If TRUE then it is assumed that the X and Z matrices are the same for GLMM in each cluster. In that case, arguments <code>x</code> and <code>z</code> have the same structure as arguments <code>x</code> and <code>z</code> of <a href="#">GLMM_MCMC</a> function. If FALSE then X and Z matrices for the GLMM may differ across clusters. In that case, arguments <code>x</code> and <code>z</code> are both lists of length equal to the number of clusters and each component of lists <code>x</code> and <code>z</code> has the same structure as arguments <code>x</code> and <code>z</code> of <a href="#">GLMM_MCMC</a> function.
<code>keep.comp.prob</code>	a logical value indicating whether the allocation probabilities should be kept for all MCMC iterations. This may ask for quite some memory but it is necessary if credible intervals etc. should be calculated for the component probabilities.
<code>level</code>	level of HPD credible intervals that are calculated for the component probabilities if <code>keep.comp.prob</code> is TRUE.
<code>info</code>	interval in which the function prints the progress of computation (unless <code>silent</code> is TRUE).
<code>silent</code>	logical value indicating whether to switch-off printing the information during calculations.

**Details**

This function complements a paper being currently in preparation.

GLMM\_longitDA2 differs in many aspects from [GLMM\\_longitDA2!](#)

**Value**

A list with the following components:

ADD	ADD DESCRIPTION
-----	-----------------

**Author(s)**

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

**See Also**

[GLMM\\_MCMC](#), [GLMM\\_longitDA](#).

**Examples**

```
### WILL BE ADDED.
```

---

GLMM\_MCMC

*MCMC estimation of a (multivariate) generalized linear mixed model with a normal mixture in the distribution of random effects*

---

**Description**

This function runs MCMC for a generalized linear mixed model with possibly several response variables and possibly normal mixtures in the distributions of random effects.

**Usage**

```
GLMM_MCMC(y, dist = "gaussian", id, x, z, random.intercept,
  prior.alpha, init.alpha, init2.alpha,
  scale.b, prior.b, init.b, init2.b,
  prior.eps, init.eps, init2.eps,
  nMCMC = c(burn = 10, keep = 10, thin = 1, info = 10),
  tuneMCMC = list(alpha = 1, b = 1),
  store = c(b = FALSE), PED = TRUE, keep.chains = TRUE,
  dens.zero = 1e-300, parallel = FALSE, cltype, silent = FALSE)
```

```
## S3 method for class 'GLMM_MCMC'
print(x, ...)
```

```
## S3 method for class 'GLMM_MCMClist'
print(x, ...)
```

**Arguments**

**y** vector, matrix or data frame with responses. If y is vector then there is only one response in the model. If y is matrix or data frame then each column gives values of one response. Missing values are allowed.

If there are several responses specified then continuous responses must be put in the first columns and discrete responses in the subsequent columns.

**dist** character (vector) which determines distribution (and a link function) for each response variable. Possible values are: "gaussian" for gaussian (normal) distribution (with identity link), "binomial(logit)" for binomial (0/1) distribution with a logit link. "poisson(log)" for Poisson distribution with a log link. Single value is recycled if necessary.

<code>id</code>	vector which determines longitudinally or otherwise dependent observations. If not given then it is assumed that there are no clusters and all observations of one response are independent.
<code>x</code>	matrix or a list of matrices with covariates (intercept not included) for fixed effects. If there is more than one response, this must always be a list. Note that intercept is included in all models. Use a character value “empty” as a component of the list <code>x</code> if there are no covariates for a particular response.
<code>z</code>	matrix or a list of matrices with covariates (intercept not included) for random effects. If there is more than one response, this must always be a list. Note that random intercept is specified using the argument <code>random.intercept</code> . <b>REMARK:</b> For a particular response, matrices <code>x</code> and <code>z</code> may not have the same columns. That is, matrix <code>x</code> includes covariates which are not involved among random effects and matrix <code>z</code> includes covariates which are involved among random effects (and implicitly among fixed effects as well).
<code>random.intercept</code>	logical (vector) which determines for which responses random intercept should be included.
<code>prior.alpha</code>	a list which specifies prior distribution for fixed effects (not the means of random effects). The prior distribution is normal and the user can specify the mean and variances. The list <code>prior.alpha</code> can have the components listed below. <b>mean</b> a vector with prior means, defaults to zeros. <b>var</b> a vector with prior variances, defaults to 10000 for all components.
<code>init.alpha</code>	a numeric vector with initial values of fixed effects (not the means of random effects) for the first chain. A sensible value is determined using the maximum-likelihood fits (using <code>lmer</code> functions) and does not have to be given by the user.
<code>init2.alpha</code>	a numeric vector with initial values of fixed effects for the second chain.
<code>scale.b</code>	a list specifying how to scale the random effects during the MCMC. A sensible value is determined using the maximum-likelihood fits (using <code>lmer</code> functions) and does not have to be given by the user. If the user wishes to influence the shift and scale constants, these are given as components of the list <code>scale.b</code> . The components are named: <b>shift</b> see vignette <a href="#">PBCseq.pdf</a> for details <b>scale</b> see vignette <a href="#">PBCseq.pdf</a> for details
<code>prior.b</code>	a list which specifies prior distribution for (shifted and scaled) random effects. The prior is in principle a normal mixture (being a simple normal distribution if we restrict the number of mixture components to be equal to one). The list <code>prior.b</code> can have the components listed below. Their meaning is analogous to the components of the same name of the argument <code>prior</code> of function <code>NMIXMCMC</code> (see therein for details). <b>distribution</b> a character string which specifies the assumed prior distribution for random effects. It can be either “normal” (multivariate normal - default) or “MVT” (multivariate Student t distribution). <b>priorK</b> a character string which specifies the type of the prior for $K$ (the number of mixture components).

	<p><b>priormuQ</b> a character string which specifies the type of the prior for mixture means and mixture variances.</p> <p><b>Kmax</b> maximal number of mixture components.</p> <p><b>lambda</b> see vignette <a href="#">PBCseq.pdf</a> for details</p> <p><b>delta</b> see vignette <a href="#">PBCseq.pdf</a> for details</p> <p><b>xi</b> see vignette <a href="#">PBCseq.pdf</a> for details</p> <p><b>ce</b> see vignette <a href="#">PBCseq.pdf</a> for details</p> <p><b>D</b> see vignette <a href="#">PBCseq.pdf</a> for details</p> <p><b>zeta</b> see vignette <a href="#">PBCseq.pdf</a> for details</p> <p><b>gD</b> see vignette <a href="#">PBCseq.pdf</a> for details</p> <p><b>hD</b> see vignette <a href="#">PBCseq.pdf</a> for details</p> <p><b>gdf</b> shape parameter of the prior distribution for the degrees of freedom if the random effects are assumed to follow the MVT distribution</p> <p><b>hdf</b> rate parameter of the prior distribution for the degrees of freedom if the random effects are assumed to follow the MVT distribution</p>
<code>init.b</code>	<p>a list with initial values of the first chain for parameters related to the distribution of random effects and random effects themselves. Sensible initial values are determined by the function itself and do not have to be given by the user.</p> <p><b>b</b></p> <p><b>K</b></p> <p><b>w</b></p> <p><b>mu</b></p> <p><b>Sigma</b></p> <p><b>Li</b></p> <p><b>gammaInv</b></p> <p><b>df</b></p> <p><b>r</b></p>
<code>init2.b</code>	<p>a list with initial values of the second chain for parameters related to the distribution of random effects and random effects themselves.</p>
<code>prior.eps</code>	<p>a list specifying prior distributions for error terms for continuous responses. The list <code>prior.eps</code> can have the components listed below. For all components, a sensible value leading to weakly informative prior distribution can be determined by the function.</p> <p><b>zeta</b> see vignette <a href="#">PBCseq.pdf</a> for details</p> <p><b>g</b> see vignette <a href="#">PBCseq.pdf</a> for details</p> <p><b>h</b> see vignette <a href="#">PBCseq.pdf</a> for details</p>
<code>init.eps</code>	<p>a list with initial values of the first chain for parameters related to the distribution of error terms of continuous responses. The list <code>init.eps</code> can have the components listed below. For all components, a sensible value can be determined by the function.</p> <p><b>sigma</b> a numeric vector with the initial values for residual standard deviations for each continuous response.</p>

	<b>gammaInv</b> a numeric vector with the initial values for the inverted components of the hyperparameter gamma for each continuous response.
init2.eps	a list with initial values of the second chain for parameters related to the distribution of error terms of continuous responses.
nMCMC	numeric vector of length 4 giving parameters of the MCMC simulation. Its components may be named (ordering is then unimportant) as: <b>burn</b> length of the burn-in (after discarding the thinned values), can be equal to zero as well. <b>keep</b> length of the kept chains (after discarding the thinned values), must be positive. <b>thin</b> thinning interval, must be positive. <b>info</b> interval in which the progress information is printed on the screen. In total $(M_{burn} + M_{keep}) \cdot M_{thin}$ MCMC scans are performed.
tuneMCMC	a list with tuning scale parameters for proposal distribution of fixed and random effects. It is used only when there are some discrete response profiles. The components of the list have the following meaning: <b>alpha</b> scale parameters by which we multiply the proposal covariance matrix when updating the fixed effects pertaining to the discrete response profiles. There is one scale parameter for each DISCRETE profile. A single value is recycled if necessary. <b>b</b> a scale parameter by which we multiply the proposal covariance matrix when updating the random effects. It is used only when there are some discrete response profiles in the model.
store	logical vector indicating whether the chains of parameters should be stored. Its components may be named (ordering is then unimportant) as: <b>b</b> if TRUE then the sampled values of random effects are stored. Defaults to FALSE.
PED	a logical value which indicates whether the penalized expected deviance (see Plummer, 2008 for more details) is to be computed (which requires two parallel chains).
keep.chains	logical. If FALSE, only summary statistics are returned in the resulting object. This might be useful in the model searching step to save some memory.
dens.zero	a small value used instead of zero when computing deviance related quantities.
parallel	a logical value which indicates whether parallel computation (based on a package parallel) should be used when running two chains for the purpose of PED calculation.
cltype	optional argument applicable if parallel is TRUE. If cltype is given, it is passed as the type argument into the call to <code>makeCluster</code> .
silent	a logical value indicating whether the information on the MCMC progress is to be suppressed.
...	additional arguments passed to the default <code>print</code> method.

## Details

See accompanying papers (Komárek et al., 2010, Komárek and Komárková, 2013).

**Value**

An object of class `GLMM_MCMClist` (if `PED` argument is `TRUE`) or `GLMM_MCMC` (if `PED` argument is `FALSE`).

**Object of class GLMM\_MCMC**

Object of class `GLMM_MCMC` can have the following components (some of them may be missing according to the context of the model):

**iter** index of the last iteration performed.

**nMCMC** used value of the argument `nMCMC`.

**dist** a character vector of length `R` corresponding to the `dist` argument.

**R** a two component vector giving the number of continuous responses and the number of discrete responses.

**p** a numeric vector of length `R` giving the number of non-intercept alpha parameters for each response.

**q** a numeric vector of length `R` giving the number of non-intercept random effects for each response.

**fixed.intercept** a logical vector of length `R` which indicates inclusion of fixed intercept for each response.

**random.intercept** a logical vector of length `R` which indicates inclusion of random intercept for each response.

**lalpha** length of the vector of fixed effects.

**dimb** dimension of the distribution of random effects.

**prior.alpha** a list containing the used value of the argument `prior.alpha`.

**prior.b** a list containing the used value of the argument `prior.b`.

**prior.eps** a list containing the used value of the argument `prior.eps`.

**init.alpha** a numeric vector with the used value of the argument `init.alpha`.

**init.b** a list containing the used value of the argument `init.b`.

**init.eps** a list containing the used value of the argument `init.eps`.

**state.first.alpha** a numeric vector with the first stored (after burn-in) value of fixed effects  $\alpha$ .

**state.last.alpha** a numeric vector with the last sampled value of fixed effects  $\alpha$ . It can be used as argument `init.alpha` to restart MCMC.

**state.first.b** a list with the first stored (after burn-in) values of parameters related to the distribution of random effects. It has components named `b`, `K`, `w`, `mu`, `Sigma`, `Li`, `Q`, `gammaInv`, `r`.

**state.last.b** a list with the last sampled values of parameters related to the distribution of random effects. It has components named `b`, `K`, `w`, `mu`, `Sigma`, `Li`, `Q`, `gammaInv`, `r`. It can be used as argument `init.b` to restart MCMC.

**state.first.eps** a list with the first stored (after burn-in) values of parameters related to the distribution of residuals of continuous responses. It has components named `sigma`, `gammaInv`.

**state.last.eps** a list with the last sampled values of parameters related to the distribution of residuals of continuous responses. It has components named `sigma`, `gammaInv`. It can be used as argument `init.eps` to restart MCMC.

- prop.accept.alpha** acceptance proportion from the Metropolis-Hastings algorithm for fixed effects (separately for each response type). Note that the acceptance proportion is equal to one for continuous responses since the Gibbs algorithm is used there.
- prop.accept.b** acceptance proportion from the Metropolis-Hastings algorithm for random effects (separately for each cluster). Note that the acceptance proportion is equal to one for models with continuous responses only since the Gibbs algorithm is used there.
- scale.b** a list containing the used value of the argument `scale.b`.
- summ.Deviance** a `data.frame` with posterior summary statistics for the deviance (approximated using the Laplacian approximation) and conditional (given random effects) deviance.
- summ.alpha** a `data.frame` with posterior summary statistics for fixed effects.
- summ.b.Mean** a matrix with posterior summary statistics for means of random effects.
- summ.b.SDCorr** a matrix with posterior summary statistics for standard deviations of random effects and correlations of each pair of random effects.
- summ.sigma\_eps** a matrix with posterior summary statistics for standard deviations of the error terms in the (mixed) models of continuous responses.
- poster.comp.prob\_u** a matrix which is present in the output object if the number of mixture components in the distribution of random effects is fixed and equal to  $K$ . In that case, `poster.comp.prob_u` is a matrix with  $K$  columns and  $I$  rows ( $I$  is the number of subjects defining the longitudinal profiles or correlated observations) with estimated posterior component probabilities – posterior means of the components of the underlying 0/1 allocation vector.  
**WARNING:** By default, the labels of components are based on artificial identifiability constraints based on ordering of the mixture means in the first margin. Very often, such identifiability constraint is not satisfactory!
- poster.comp.prob\_b** a matrix which is present in the output object if the number of mixture components in the distribution of random effects is fixed and equal to  $K$ . In that case, `poster.comp.prob_b` is a matrix with  $K$  columns and  $I$  rows ( $I$  is the number of subjects defining the longitudinal profiles or correlated observations) with estimated posterior component probabilities – posterior mean over model parameters including random effects.  
**WARNING:** By default, the labels of components are based on artificial identifiability constraints based on ordering of the mixture means in the first margin. Very often, such identifiability constraint is not satisfactory!
- freqK\_b** frequency table for the MCMC sample of the number of mixture components in the distribution of the random effects.
- propK\_b** posterior probabilities for the numbers of mixture components in the distribution of random effects.
- poster.mean.y** a list with `data.frames`, one `data.frame` per response profile. Each `data.frame` with columns labeled `id`, `observed`, `fitted`, `stres`, `eta.fixed` and `eta.random` holding identifier for clusters of grouped observations, observed values and posterior means for fitted values (response expectation given fixed and random effects), standardized residuals (derived from fitted values), fixed effect part of the linear predictor and the random effect part of the linear predictor. In each column, there are first all values for the first response, then all values for the second response etc.
- poster.mean.profile** a `data.frame` with columns labeled `b1`, ..., `bq`, `Logpb`, `Cond.Deviance`, `Deviance` with posterior means of random effects for each cluster, posterior means of  $\log\{p(\mathbf{b})\}$ ,



conditional deviances, i.e., minus twice the conditional (given random effects) log-likelihood for each cluster and GLMM deviances, i.e., minus twice the marginal (random effects integrated out) log-likelihoods for each cluster. The value of the marginal (random effects integrated out) log-likelihood at each MCMC iteration is obtained using the Laplacian approximation.

**poster.mean.w\_b** a numeric vector with posterior means of mixture weights after re-labeling. It is computed only if  $K_b$  is fixed and even then I am not convinced that these are useful posterior summary statistics (see label switching problem mentioned above). In any case, they should be used with care.

**poster.mean.mu\_b** a matrix with posterior means of mixture means after re-labeling. It is computed only if  $K_b$  is fixed and even then I am not convinced that these are useful posterior summary statistics (see label switching problem mentioned above). In any case, they should be used with care.

**poster.mean.Q\_b** a list with posterior means of mixture inverse variances after re-labeling. It is computed only if  $K_b$  is fixed and even then I am not convinced that these are useful posterior summary statistics (see label switching problem mentioned above). In any case, they should be used with care.

**poster.mean.Sigma\_b** a list with posterior means of mixture variances after re-labeling. It is computed only if  $K_b$  is fixed and even then I am not convinced that these are useful posterior summary statistics (see label switching problem mentioned above). In any case, they should be used with care.

**poster.mean.Li\_b** a list with posterior means of Cholesky decompositions of mixture inverse variances after re-labeling. It is computed only if  $K_b$  is fixed and even then I am not convinced that these are useful posterior summary statistics (see label switching problem mentioned above). In any case, they should be used with care.

**Deviance** numeric vector with a chain for the GLMM deviances, i.e., twice the marginal (random effects integrated out) log-likelihoods of the GLMM. The marginal log-likelihood is obtained using the Laplacian approximation at each iteration of MCMC.

**Cond.Deviance** numeric vector with a chain for the conditional deviances, i.e., twice the conditional (given random effects) log-likelihoods.

**K\_b** numeric vector with a chain for  $K_b$  (number of mixture components in the distribution of random effects).

**w\_b** numeric vector or matrix with a chain for  $w_b$  (mixture weights for the distribution of random effects). It is a matrix with  $K_b$  columns when  $K_b$  is fixed. Otherwise, it is a vector with weights put sequentially after each other.

**mu\_b** numeric vector or matrix with a chain for  $\mu_b$  (mixture means for the distribution of random effects). It is a matrix with  $dimb \cdot K_b$  columns when  $K_b$  is fixed. Otherwise, it is a vector with means put sequentially after each other.

**Q\_b** numeric vector or matrix with a chain for lower triangles of  $Q_b$  (mixture inverse variances for the distribution of random effects). It is a matrix with  $\frac{dimb(dimb+1)}{2} \cdot K_b$  columns when  $K_b$  is fixed. Otherwise, it is a vector with lower triangles of  $Q_b$  matrices put sequentially after each other.

**Sigma\_b** numeric vector or matrix with a chain for lower triangles of  $\Sigma_b$  (mixture variances for the distribution of random effects). It is a matrix with  $\frac{dimb(dimb+1)}{2} \cdot K_b$  columns when  $K_b$  is fixed. Otherwise, it is a vector with lower triangles of  $\Sigma_b$  matrices put sequentially after each other.

- Li\_b** numeric vector or matrix with a chain for lower triangles of Cholesky decompositions of  $Q_b$  matrices. It is a matrix with  $\frac{dimb(dimb+1)}{2} \cdot K_b$  columns when  $K_b$  is fixed. Otherwise, it is a vector with lower triangles put sequentially after each other.
- gammaInv\_b** matrix with  $dimb$  columns with a chain for inverses of the hyperparameter  $\gamma_b$ .
- order\_b** numeric vector or matrix with order indeces of mixture components in the distribution of random effects related to artificial identifiability constraint defined by ordering of the first component of the mixture means.  
It is a matrix with  $K_b$  columns when  $K_b$  is fixed. Otherwise it is a vector with orders put sequentially after each other.
- rank\_b** numeric vector or matrix with rank indeces of mixture components in the distribution of random effects related to artificial identifiability constraint defined by ordering of the first component of the mixture means.  
It is a matrix with  $K_b$  columns when  $K_b$  is fixed. Otherwise it is a vector with ranks put sequentially after each other.
- mixture\_b** data.frame with columns labeled b.Mean.\*, b.SD.\*, b.Corr.\*.\* containing the chains for the means, standard deviations and correlations of the distribution of the random effects based on a normal mixture at each iteration.
- b** a matrix with the MCMC chains for random effects. It is included only if store[b] is TRUE.
- alpha** numeric vector or matrix with the MCMC chain(s) for fixed effects.
- sigma\_eps** numeric vector or matrix with the MCMC chain(s) for standard deviations of the error terms in the (mixed) models for continuous responses.
- gammaInv\_eps** matrix with  $dimb$  columns with MCMC chain(s) for inverses of the hyperparameter  $\gamma_b$ .
- relabel\_b** a list which specifies the algorithm used to re-label the MCMC output to compute order\_b, rank\_b, poster.comp.prob\_u, poster.comp.prob\_b, poster.mean.w\_b, poster.mean.mu\_b, poster.mean.Q\_b, poster.mean.Sigma\_b, poster.mean.Li\_b.
- Cpar** a list with components useful to call underlying C++ functions (not interesting for ordinary users).

### Object of class GLMM\_MCMClist

Object of class NMixMCMClist is the list having two components of class NMixMCMC representing two parallel chains and additionally the following components:

- PED** values of penalized expected deviance and related quantities. It is a vector with five components: D.expect = estimated expected deviance, where the estimate is based on two parallel chains; popt = estimated penalty, where the estimate is based on simple MCMC average based on two parallel chains; PED = estimated penalized expected deviance = D.expect + popt; wpopt = estimated penalty, where the estimate is based on weighted MCMC average (through importance sampling) based on two parallel chains; wPED = estimated penalized expected deviance = D.expect + wpopt.
- D** posterior mean of the deviance for each subject.
- popt** contributions to the unweighted penalty from each subject.
- wpopt** contributions to the weighted penalty from each subject.

- inv.D** for each subject, number of iterations (in both chains), where the deviance was in fact equal to infinity (when the corresponding density was lower than `dens.zero`) and was not taken into account when computing `D.expect`.
- inv.popt** for each subject, number of iterations, where the penalty was in fact equal to infinity and was not taken into account when computing `popt`.
- inv.wpopt** for each subject, number of iterations, where the importance sampling weight was in fact equal to infinity and was not taken into account when computing `wpopt`.
- sumISw** for each subject, sum of importance sampling weights.
- Deviance1** sampled value of the observed data deviance from chain 1
- Deviance2** sampled values of the observed data deviance from chain 2
- Deviance\_repl1\_ch1** sampled values of the deviance of data replicated according to the chain 1 evaluated under the parameters from chain 1
- Deviance\_repl1\_ch2** sampled values of the deviance of data replicated according to the chain 1 evaluated under the parameters from chain 2
- Deviance\_repl2\_ch1** sampled values of the deviance of data replicated according to the chain 2 evaluated under the parameters from chain 1
- Deviance\_repl2\_ch2** sampled values of the deviance of data replicated according to the chain 2 evaluated under the parameters from chain 2

#### Author(s)

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

#### References

- Komárek, A. and Komárková, L. (2013). Clustering for multivariate continuous and discrete longitudinal data. *The Annals of Applied Statistics*, **7**(1), 177–200.
- Komárek, A. and Komárková, L. (2014). Capabilities of R package `mixAK` for clustering based on multivariate continuous and discrete longitudinal data. *Journal of Statistical Software*, **59**(12), 1–38. <http://www.jstatsoft.org/v59/i12/>.
- Komárek, A., Hansen, B. E., Kuiper, E. M. M., van Buuren, H. R., and Lesaffre, E. (2010). Discriminant analysis using a multivariate linear mixed model with a normal mixture in the random effects distribution. *Statistics in Medicine*, **29**(30), 3267–3283.
- Plummer, M. (2008). Penalized loss functions for Bayesian model comparison. *Biostatistics*, **9**(3), 523–539.

#### See Also

[NMixMCMC](#).

#### Examples

```
## See also additional material available in
## YOUR_R_DIR/library/mixAK/doc/
## or YOUR_R_DIR/site-library/mixAK/doc/
## - files http://www.karlin.mff.cuni.cz/~komarek/software/mixAK/PBCseq.pdf,
```

```
##          PBCseq.R
## =====
```

---

MatMPpinv                      *Moore-Penrose pseudoinverse of a squared matrix*

---

### Description

For a matrix  $A$  its Moore-Penrose pseudoinverse is such a matrix  $A^+$  which satisfies

- (i)  $AA^+A = A$ ,
- (ii)  $A^+AA^+ = A^+$ ,
- (iii)  $(AA^+)' = AA^+$ ,
- (iv)  $(A^+A) = A^+A$ .

Computation is done using spectral decomposition. At this moment, it is implemented for symmetric matrices only.

### Usage

```
MatMPpinv(A)
```

### Arguments

$A$                       either a numeric vector in which case inverse of each element of  $A$  is returned or a squared matrix.

### Value

Either a numeric vector or a matrix.

### Author(s)

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

### References

Golub, G. H. and Van Loan, C. F. (1996, Sec. 5.5). *Matrix Computations. Third Edition*. Baltimore: The Johns Hopkins University Press.

### Examples

```
set.seed(770328)
A <- rWISHART(1, 5, diag(4))
Ainv <- MatMPpinv(A)

### Check the conditions
```

```

prec <- 13
round(A - A %% Ainv %% A, prec)
round(Ainv - Ainv %% A %% Ainv, prec)
round(A %% Ainv - t(A %% Ainv), prec)
round(Ainv %% A - t(Ainv %% A), prec)

```

---

MatSqrt

*Square root of a matrix*


---

### Description

For a matrix  $A$  its square root is such a matrix  $B$  which satisfies  $A = BB$ .

Computation is done using spectral decomposition. When calculating the square roots of eigenvalues, always a root with positive real part and a sign of the imaginary part the same as the sign of the imaginary eigenvalue part is taken.

### Usage

```
MatSqrt(A)
```

### Arguments

$A$  either a numeric vector in which case square roots of each element of  $A$  is returned or a squared matrix.

### Value

Either a numeric vector or a matrix.

### Author(s)

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

### Examples

```

MatSqrt(0:4)
MatSqrt((-4):0)
MatSqrt(c(-1, 1, -2, 2))

A <- (1:4) %% t(1:4)
sqrtA <- MatSqrt(A)
sqrtA
round(sqrtA %% sqrtA - A, 13)

### The following example crashes on r-devel Windows x64 x86_64,
### on r-patched Linux x86_64
### due to failure of LAPACK zgesv routine
###
### Commented on 16/01/2010

```

```

###
# B <- -A
# sqrtB <- MatSqrt(B)
# sqrtB
# round(Re(sqrtB %*% sqrtB - B), 13)
# round(Im(sqrtB %*% sqrtB - B), 13)

V <- eigen(A)$vectors
sqrtV <- MatSqrt(V)
sqrtV
round(sqrtV %*% sqrtV - V, 14)

Sigma <- matrix(c(1, 1, 1.5, 1, 4, 4.2, 1.5, 4.2, 9), nrow=3)
sqrtSigma <- MatSqrt(Sigma)
sqrtSigma
round(sqrtSigma %*% sqrtSigma - Sigma, 13)

D4 <- matrix(c(5, -4, 1, 0, 0,
               -4, 6, -4, 1, 0,
               1, -4, 6, -4, 1,
               0, 1, -4, 6, -4,
               0, 0, 1, -4, 5), nrow=5)
sqrtD4 <- MatSqrt(D4)
sqrtD4[abs(sqrtD4) < 1e-15] <- 0
sqrtD4
round(sqrtD4 %*% sqrtD4 - D4, 14)

X <- matrix(c(7, 15, 10, 22), nrow=2)
sqrtX <- MatSqrt(X)
sqrtX %*% sqrtX - X

```

---

 MVN

*Multivariate normal distribution*


---

### Description

Density and random generation for the multivariate normal distribution with mean equal to mean, precision matrix equal to Q (or covariance matrix equal to Sigma).

Function `rcMVN` samples from the multivariate normal distribution with a canonical mean  $b$ , i.e., the mean is  $\mu = Q^{-1} b$ .

### Usage

```
dMVN(x, mean=0, Q=1, Sigma, log=FALSE)
```

```
rMVN(n, mean=0, Q=1, Sigma)
```

```
rcMVN(n, b=0, Q=1, Sigma)
```

**Arguments**

mean	vector of mean.
b	vector of a canonical mean.
Q	precision matrix of the multivariate normal distribution. Ignored if Sigma is given.
Sigma	covariance matrix of the multivariate normal distribution. If Sigma is supplied, precision is computed from $\Sigma$ as $Q = \Sigma^{-1}$ .
n	number of observations to be sampled.
x	vector or matrix of the points where the density should be evaluated.
log	logical; if TRUE, log-density is computed

**Value**

Some objects.

**Value for dMVN**

A vector with evaluated values of the (log-)density

**Value for rMVN**

A list with the components:

**x** vector or matrix with sampled values

**log.dens** vector with the values of the log-density evaluated in the sampled values

**Value for rcMVN**

A list with the components:

**x** vector or matrix with sampled values

**mean** vector or the mean of the normal distribution

**log.dens** vector with the values of the log-density evaluated in the sampled values

**Author(s)**

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

**References**

Rue, H. and Held, L. (2005). *Gaussian Markov Random Fields: Theory and Applications*. Boca Raton: Chapman and Hall/CRC.

**See Also**

[dnorm](#), [Mvnorm](#).

**Examples**

```

set.seed(1977)

### Univariate normal distribution
### =====
c(dMVN(0), dnorm(0))
c(dMVN(0, log=TRUE), dnorm(0, log=TRUE))

rbind(dMVN(c(-1, 0, 1)), dnorm(c(-1, 0, 1)))
rbind(dMVN(c(-1, 0, 1), log=TRUE), dnorm(c(-1, 0, 1), log=TRUE))

c(dMVN(1, mean=1.2, Q=0.5), dnorm(1, mean=1.2, sd=sqrt(2)))
c(dMVN(1, mean=1.2, Q=0.5, log=TRUE), dnorm(1, mean=1.2, sd=sqrt(2), log=TRUE))

rbind(dMVN(0:2, mean=1.2, Q=0.5), dnorm(0:2, mean=1.2, sd=sqrt(2)))
rbind(dMVN(0:2, mean=1.2, Q=0.5, log=TRUE), dnorm(0:2, mean=1.2, sd=sqrt(2), log=TRUE))

### Multivariate normal distribution
### =====
mu <- c(0, 6, 8)
L <- matrix(1:9, nrow=3)
L[upper.tri(L, diag=FALSE)] <- 0
Sigma <- L %*% t(L)
Q <- chol2inv(chol(Sigma))
b <- solve(Sigma, mu)

dMVN(mu, mean=mu, Q=Q)
dMVN(mu, mean=mu, Sigma=Sigma)
dMVN(mu, mean=mu, Q=Q, log=TRUE)
dMVN(mu, mean=mu, Sigma=Sigma, log=TRUE)

xx <- matrix(c(0,6,8, 1,5,7, -0.5,5.5,8.5, 0.5,6.5,7.5), ncol=3, byrow=TRUE)
dMVN(xx, mean=mu, Q=Q)
dMVN(xx, mean=mu, Sigma=Sigma)
dMVN(xx, mean=mu, Q=Q, log=TRUE)
dMVN(xx, mean=mu, Sigma=Sigma, log=TRUE)

zz <- rMVN(1000, mean=mu, Sigma=Sigma)
rbind(apply(zz$x, 2, mean), mu)
var(zz$x)
Sigma
cbind(dMVN(zz$x, mean=mu, Sigma=Sigma, log=TRUE), zz$log.dens)[1:10,]

zz <- rcMVN(1000, b=b, Sigma=Sigma)
rbind(apply(zz$x, 2, mean), mu)
var(zz$x)
Sigma
cbind(dMVN(zz$x, mean=mu, Sigma=Sigma, log=TRUE), zz$log.dens)[1:10,]

zz <- rMVN(1000, mean=rep(0, 3), Sigma=Sigma)
rbind(apply(zz$x, 2, mean), rep(0, 3))
var(zz$x)

```



```

Sigma
cbind(dMVN(zz$x, mean=rep(0, 3), Sigma=Sigma, log=TRUE), zz$log.dens)[1:10,]

### The same using the package mvtnorm
### =====
# require(mvtnorm)
# c(dMVN(mu, mean=mu, Sigma=Sigma), dmvnorm(mu, mean=mu, sigma=Sigma))
# c(dMVN(mu, mean=mu, Sigma=Sigma, log=TRUE), dmvnorm(mu, mean=mu, sigma=Sigma, log=TRUE))
#
# rbind(dMVN(xx, mean=mu, Sigma=Sigma), dmvnorm(xx, mean=mu, sigma=Sigma))
# rbind(dMVN(xx, mean=mu, Sigma=Sigma, log=TRUE), dmvnorm(xx, mean=mu, sigma=Sigma, log=TRUE))

```

---

MVNmixture

*Mixture of (multivariate) normal distributions*


---

### Description

Density and random generation for the mixture of the  $p$ -variate normal distributions with means given by mean, precision matrix given by Q (or covariance matrices given by Sigma).

### Usage

```
dMVNmixture(x, weight, mean, Q, Sigma, log=FALSE)
```

```
dMVNmixture2(x, weight, mean, Q, Sigma, log=FALSE)
```

```
rMVNmixture(n, weight, mean, Q, Sigma)
```

```
rMVNmixture2(n, weight, mean, Q, Sigma)
```

### Arguments

weight	vector of length $K$ with the mixture weights or values which are proportional to the weights.
mean	vector or matrix of mixture means. For $p = 1$ this should be a vector of length $K$ , for $p > 1$ this should be a $K \times p$ matrix with mixture means in rows.
Q	precision matrices of the multivariate normal distribution. Ignored if Sigma is given. For $p = 1$ this should be a vector of length $K$ , for $p > 1$ this should be a list of length $K$ with the mixture precision matrices as components of the list.
Sigma	covariance matrix of the multivariate normal distribution. If Sigma is supplied, precisions are computed from $\Sigma$ as $Q = \Sigma^{-1}$ . For $p = 1$ this should be a vector of length $K$ , for $p > 1$ this should be a list of length $K$ with the mixture covariance matrices as components of the list.

n	number of observations to be sampled.
x	vector or matrix of the points where the density should be evaluated.
log	logical; if TRUE, log-density is computed

### Details

Functions `dMVNmixture` and `dMVNmixture2` differ only internally in the way they compute the mixture density. In `dMVNmixture`, only multivariate normal densities are evaluated in compiled C++ code and mixing is done directly in R. In `dMVNmixture2`, everything is evaluated in compiled C++ code. Normally, both `dMVNmixture` and `dMVNmixture2` should return the same results.

Similarly for `rMVNmixture` and `rMVNmixture2`. Another difference is that `rMVNmixture` returns only random generated points and `rMVNmixture2` also values of the density evaluated in the generated points.

### Value

Some objects.

### Value for `dMVNmixture`

A vector with evaluated values of the (log-)density.

### Value for `dMVNmixture2`

A vector with evaluated values of the (log-)density.

### Value for `rMVNmixture`

A vector (for  $n=1$  or for univariate mixture) or matrix with sampled values (in rows of the matrix).

### Value for `rMVNmixture2`

A list with components named `x` which is a vector (for  $n=1$  or for univariate mixture) or matrix with sampled values (in rows of the matrix) and `dens` which are the values of the density evaluated in `x`.

### Author(s)

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

### See Also

[dnorm](#), [MVN](#), [Mvnorm](#).

## Examples

```

set.seed(1977)

##### Univariate normal mixture
##### =====
mu <- c(-1, 1)
Sigma <- c(0.25^2, 0.4^2)
Q <- 1/Sigma
w <- c(0.3, 0.7)

xx <- seq(-2, 2.5, length=100)
yyA <- dMVNmixture(xx, weight=w, mean=mu, Sigma=Sigma)
yyB <- dMVNmixture(xx, weight=w, mean=mu, Q=Q)
yyC <- dMVNmixture2(xx, weight=w, mean=mu, Sigma=Sigma)
yyD <- dMVNmixture2(xx, weight=w, mean=mu, Q=Q)

xxSample <- rMVNmixture(1000, weight=w, mean=mu, Sigma=Sigma)
xxSample2 <- rMVNmixture2(1000, weight=w, mean=mu, Sigma=Sigma)

sum(abs(xxSample2$dens - dMVNmixture(xxSample2$x, weight=w, mean=mu, Sigma=Sigma)) > 1e-15)
xxSample2 <- xxSample2$x

par(mfrow=c(2, 2), bty="n")
plot(xx, yyA, type="l", col="red", xlab="x", ylab="f(x)")
points(xx, yyB, col="darkblue")
hist(xxSample, col="lightblue", prob=TRUE, xlab="x", xlim=range(xx), ylim=c(0, max(yyA)),
      main="Sampled values")
lines(xx, yyA, col="red")
plot(xx, yyC, type="l", col="red", xlab="x", ylab="f(x)")
points(xx, yyD, col="darkblue")
hist(xxSample2, col="sandybrown", prob=TRUE, xlab="x", xlim=range(xx), ylim=c(0, max(yyA)),
      main="Sampled values")
lines(xx, yyC, col="red")

##### Bivariate normal mixture
##### =====
### Choice 1
sd11 <- sd12 <- 1.1
sd21 <- 0.5
sd22 <- 1.5
rho2 <- 0.7
Xlim <- c(-3, 4)
Ylim <- c(-6, 4)

### Choice 2
sd11 <- sd12 <- 0.3
sd21 <- 0.5
sd22 <- 0.3
rho2 <- 0.8
Xlim <- c(-3, 2.5)
Ylim <- c(-2.5, 2.5)

```

```

mu <- matrix(c(1,1, -1,-1), nrow=2, byrow=TRUE)
Sigma <- list(diag(c(sd11^2, sd12^2)),
             matrix(c(sd21^2, rho2*sd21*sd22, rho2*sd21*sd22, sd22^2), nrow=2))
Q <- list(chol2inv(chol(Sigma[[1]])), chol2inv(chol(Sigma[[2]])))
w <- c(0.3, 0.7)

xx1 <- seq(mu[2,1]-3*sd21, mu[1,1]+3*sd11, length=100)
xx2 <- seq(mu[2,2]-3*sd22, mu[1,2]+3*sd12, length=90)
XX <- cbind(rep(xx1, length(xx2)), rep(xx2, each=length(xx1)))
yyA <- matrix(dMVNmixture(XX, weight=w, mean=mu, Sigma=Sigma), nrow=length(xx1), ncol=length(xx2))
yyB <- matrix(dMVNmixture(XX, weight=w, mean=mu, Q=Q), nrow=length(xx1), ncol=length(xx2))
yyC <- matrix(dMVNmixture2(XX, weight=w, mean=mu, Sigma=Sigma), nrow=length(xx1), ncol=length(xx2))
yyD <- matrix(dMVNmixture2(XX, weight=w, mean=mu, Q=Q), nrow=length(xx1), ncol=length(xx2))

#xxSample <- rMVNmixture(1000, weight=w, mean=mu, Sigma=Sigma)
### Starting from version 3.6, the above command led to SegFault
### on CRAN r-patched-solaris-sparc check.
### Commented here on 20140806 (version 3.6-1).
xxSample2 <- rMVNmixture2(1000, weight=w, mean=mu, Sigma=Sigma)

sum(abs(xxSample2$dens - dMVNmixture(xxSample2$x, weight=w, mean=mu, Sigma=Sigma)) > 1e-15)
xxSample2 <- xxSample2$x

par(mfrow=c(1, 2), bty="n")
plot(xxSample, col="darkblue", xlab="x1", ylab="x2", xlim=Xlim, ylim=Ylim)
contour(xx1, xx2, yyA, col="red", add=TRUE)
plot(xxSample2, col="darkblue", xlab="x1", ylab="x2", xlim=Xlim, ylim=Ylim)
contour(xx1, xx2, yyC, col="red", add=TRUE)

par(mfrow=c(2, 2), bty="n")
contour(xx1, xx2, yyA, col="red", xlab="x1", ylab="x2")
points(mu[,1], mu[,2], col="darkgreen")
persp(xx1, xx2, yyA, col="lightblue", xlab="x1", ylab="x2", zlab="f(x1, x2)")
contour(xx1, xx2, yyB, col="red", xlab="x1", ylab="x2")
points(mu[,1], mu[,2], col="darkgreen")
persp(xx1, xx2, yyB, col="lightblue", xlab="x1", ylab="x2", zlab="f(x1, x2)", phi=30, theta=30)

par(mfrow=c(2, 2), bty="n")
contour(xx1, xx2, yyC, col="red", xlab="x1", ylab="x2")
points(mu[,1], mu[,2], col="darkgreen")
persp(xx1, xx2, yyC, col="lightblue", xlab="x1", ylab="x2", zlab="f(x1, x2)")
contour(xx1, xx2, yyD, col="red", xlab="x1", ylab="x2")
points(mu[,1], mu[,2], col="darkgreen")
persp(xx1, xx2, yyD, col="lightblue", xlab="x1", ylab="x2", zlab="f(x1, x2)", phi=30, theta=30)

```

**Description**

Density and random generation for the multivariate Student t distribution with location equal to  $\mu$ , precision matrix equal to  $Q$  (or scale matrix equal to  $\Sigma$ ).

Mentioned functions implement the multivariate Student t distribution with a density given by

$$p(\mathbf{z}) = \frac{\Gamma\left(\frac{\nu+p}{2}\right)}{\Gamma\left(\frac{\nu}{2}\right) \nu^{\frac{p}{2}} \pi^{\frac{p}{2}}} |\Sigma|^{-\frac{1}{2}} \left\{ 1 + \frac{(\mathbf{z} - \boldsymbol{\mu})' \Sigma^{-1} (\mathbf{z} - \boldsymbol{\mu})}{\nu} \right\}^{-\frac{\nu+p}{2}},$$

where  $p$  is the dimension,  $\nu > 0$  degrees of freedom,  $\boldsymbol{\mu}$  the location parameter and  $\Sigma$  the scale matrix.

For  $\nu > 1$ , the mean is equal to  $\boldsymbol{\mu}$ , for  $\nu > 2$ , the covariance matrix is equal to  $\frac{\nu}{\nu-2} \Sigma$ .

**Usage**

```
dMVT(x, df, mu=0, Q=1, Sigma, log=FALSE)
```

```
rMVT(n, df, mu=0, Q=1, Sigma)
```

**Arguments**

df	degrees of freedom of the multivariate Student t distribution.
mu	vector of the location parameter.
Q	precision (inverted scale) matrix of the multivariate Student t distribution. Ignored if Sigma is given.
Sigma	scale matrix of the multivariate Student t distribution. If Sigma is supplied, precision is computed from $\Sigma$ as $Q = \Sigma^{-1}$ .
n	number of observations to be sampled.
x	vector or matrix of the points where the density should be evaluated.
log	logical; if TRUE, log-density is computed

**Value**

Some objects.

**Value for dMVT**

A vector with evaluated values of the (log-)density

**Value for rMVT**

A list with the components:

**x** vector or matrix with sampled values

**log.dens** vector with the values of the log-density evaluated in the sampled values

**Author(s)**

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

**See Also**

[dt](#), [Mvt](#).

**Examples**

```
set.seed(1977)

### Univariate central t distribution
z <- rMVT(10, df=1, mu=0, Q=1)
ldz <- dMVT(z$x, df=1, log=TRUE)
boxplot(as.numeric(z$x))
cbind(z$log.dens, ldz, dt(as.numeric(z$x), df=1, log=TRUE))

### Multivariate t distribution
mu <- c(1, 2, 3)
Sigma <- matrix(c(1, 1, -1.5, 1, 4, 1.8, -1.5, 1.8, 9), nrow=3)
Q <- chol2inv(chol(Sigma))

nu <- 3
z <- rMVT(1000, df=nu, mu=mu, Sigma=Sigma)
apply(z$x, 2, mean)      ## should be close to mu
((nu - 2) / nu) * var(z$x)  ## should be close to Sigma

dz <- dMVT(z$x, df=nu, mu=mu, Sigma=Sigma)
ldz <- dMVT(z$x, df=nu, mu=mu, Sigma=Sigma, log=TRUE)

### Compare with mvtnorm package
#require(mvtnorm)
#ldz2 <- dmvt(z$x, sigma=Sigma, df=nu, delta=mu, log=TRUE)
#plot(z$log.dens, ldz2, pch=21, col="red3", bg="orange", xlab="mixAK", ylab="mvtnorm")
#plot(ldz, ldz2, pch=21, col="red3", bg="orange", xlab="mixAK", ylab="mvtnorm")
```

---

NMixChainComp

*Chains for mixture parameters*

---

**Description**

This function returns chains for parameters derived from the (re-labeled) mixture weights, means, covariance matrices.

First, mixture means and shifted-scaled to the original (data) scale, mixture covariance matrices are scaled to the original (data) scale (see argument `scale` in [NMixMCMC](#) function or argument `scale.b` in [GLMM\\_MCMC](#)). Possible derived parameters are standard deviations and correlation coefficients.

**Usage**

```
NMixChainComp(x, relabel = TRUE, param)
```

```
## Default S3 method:
```

```

NMixChainComp(x, relabel = TRUE, param)

## S3 method for class 'NMixMCMC'
NMixChainComp(x, relabel = TRUE,
  param = c("w", "mu", "var", "sd", "cor", "Sigma", "Q", "Li"))

## S3 method for class 'GLMM_MCMC'
NMixChainComp(x, relabel = TRUE,
  param = c("w_b", "mu_b", "var_b", "sd_b", "cor_b", "Sigma_b", "Q_b", "Li_b"))

```

### Arguments

<code>x</code>	an object of class <code>NMIXMCMC</code> or <code>GLMM_MCMC</code> .
<code>relabel</code>	a logical argument indicating whether the chains are to be returned with components being re-labeled (see <a href="#">NMixRelabel</a> ) or whether the chains are to be returned as originally sampled.
<code>param</code>	a character string indicating which sample is to be returned: <b>w, w_b</b> mixture weights; <b>mu, mu_b</b> mixture means; <b>var, var_b</b> mixture variances; <b>sd, sd_b</b> mixture standard deviations; <b>cor, cor_b</b> correlations derived from the mixture covariance matrices; <b>Sigma, Sigma_b</b> mixture covariance matrices (their lower triangles); <b>Q, Q_b</b> mixture inverted covariance matrices (their lower triangles); <b>Li, Li_b</b> Cholesky factors (their lower triangles) of the mixture inverted covariance matrices.

### Value

A matrix with sampled values in rows, parameters in columns.

### Author(s)

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

### See Also

[NMixMCMC](#), [GLMM\\_MCMC](#).

---

NMixChainsDerived	<i>Create MCMC chains derived from previously sampled values</i>
-------------------	--

---

## Description

Currently, this function creates chains for marginal means of  $\exp(\text{data})$  from previously sampled values (see [NMixMCMC](#)). This is useful in survival context when a density of  $Y = \log(T)$  is modelled using the function [NMixMCMC](#) and we are interested in inference on  $ET = E \exp(Y)$ .

## Usage

```
NMixChainsDerived(object)
```

## Arguments

`object` an object of class `NMixMCMC` or `NMixMCMClist`

## Value

An object of the same class as argument `object`. When `object` was of class `NMixMCMC`, the resulting object contains additionally the following components:

`chains.derived` a `data.frame` with columns labeled `expy.Mean.1, ..., expy.Mean.p` containing the sampled values of  $E \exp(Y_1), \dots, E \exp(Y_p)$ .

`summ.expy.Mean` posterior summary statistics for  $E \exp(Y_1), \dots, E \exp(Y_p)$ .

When `object` was of the class `NMixMCMClist` then each of its components (`chains`) is augmented by new components `chains.derived` and `summ.expy.Mean`.

## Author(s)

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

## See Also

[NMixMCMC](#).



---

 NMixCluster

*Clustering based on the MCMC output of the mixture model*


---

**Description**

TO BE ADDED.

This function only works for models with a fixed number of mixture components.

**Usage**

```

NMixCluster(object, ...)

## Default S3 method:
NMixCluster(object, ...)

## S3 method for class 'GLMM_MCMC'
NMixCluster(object,
  prob = c("poster.comp.prob", "quant.comp.prob", "poster.comp.prob_b",
           "quant.comp.prob_b", "poster.comp.prob_u"),
  pquant = 0.5, HPD = FALSE, pHPD = 0.95, pthresh = -1, unclass.na = FALSE, ...)

```

**Arguments**

object	an object of appropriate class.
prob	character string which identifies estimates of the component probabilities to be used for clustering.
pquant	when prob is either “quant.comp.prob” or “quant.comp.prob_b”, argument pquant is the probability of the quantile of the component probabilities to be used for clustering.
HPD	logical value. If TRUE then only those subjects are classified for which the lower limit of the $pHPD \cdot 100\%$ HPD credible interval of the component probability exceeds the value of ptrash.
pHPD	credible level of the HPD credible interval, see argument HPD.
pthresh	an optional threshold for the estimated component probability (when HPD is FALSE) or for the lower limit of the HPD credible interval (when HPD is TRUE) to classify a subject. No effect when pthresh is negative.
unclass.na	logical value taken into account when pthresh is positive. If unclass.na is TRUE, unclassified subjects get classification NA. If unclass.na is FALSE, unclassified subjects create a separate (last) group.
...	optional additional arguments.

**Value**

A data.frame with three (when HPD is FALSE) or five (when HPD is TRUE) columns.

**Author(s)**

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

**See Also**

[NMixMCMC](#), [GLMM\\_MCMC](#).

**Examples**

```
## TO BE ADDED.
```

---

NMixEM

*EM algorithm for a homoscedastic normal mixture*

---

**Description**

This function computes ML estimates of the parameters of the  $p$ -dimensional  $K$ -component normal mixture using the EM algorithm

**Usage**

```
NMixEM(y, K, weight, mean, Sigma, toler=1e-5, maxiter=500)
```

```
## S3 method for class 'NMixEM'
print(x, ...)
```

**Arguments**

y	vector (if $p = 1$ ) matrix or data frame (if $p > 1$ ) with data. Rows correspond to observations, columns correspond to margins.
K	required number of mixture components.
weight	a numeric vector with initial mixture weights. If not given, initial weights are all equal to $1/K$ .
mean	vector or matrix of initial mixture means. For $p = 1$ this should be a vector of length $K$ , for $p > 1$ this should be a $K \times p$ matrix with mixture means in rows.
Sigma	number or $p \times p$ matrix giving the initial variance/covariance matrix.
toler	tolerance to determine convergence.
maxiter	maximum number of iterations of the EM algorithm.
x	an object of class NMixEM.
...	additional arguments passed to the default print method.

**Value**

An object of class NMixEM which has the following components:

K	number of mixture components
weight	estimated mixture weights
mean	estimated mixture means
Sigma	estimated covariance matrix
loglik	log-likelihood value at fitted values
aic	Akaike information criterion $(-2\hat{\ell} + 2\nu)$ , where $\hat{\ell}$ stands for the log-likelihood value at fitted values and $\nu$ for the number of free model parameters
bic	Bayesian (Schwarz) information criterion $(-2\hat{\ell} + \log(n)\nu)$ , where $\hat{\ell}$ stands for the log-likelihood value at fitted values and $\nu$ for the number of free model parameters, and $n$ for the sample size
iter	number of iterations of the EM algorithm used to get the solution
iter.loglik	values of the log-likelihood at iterations of the EM algorithm
iter.Qfun	values of the EM objective function at iterations of the EM algorithm
dim	dimension $p$
nobs	number of observations $n$

**Author(s)**

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

**References**

Dempster, A. P., Laird, N. M., Rubin, D. B. (1977). Maximum likelihood from incomplete data via the EM algorithm. *Journal of the Royal Statistical Society, Series B*, **39**, 1-38.

**Examples**

```
## Not run:
## Estimates for 3-component mixture in Anderson's iris data
## =====
data(iris, package="datasets")
summary(iris)

VARS <- names(iris)[1:4]
fit <- NMixEM(iris[, VARS], K = 3)
print(fit)

apply(subset(iris, Species == "versicolor")[, VARS], 2, mean)
apply(subset(iris, Species == "setosa")[, VARS], 2, mean)
apply(subset(iris, Species == "virginica")[, VARS], 2, mean)

## Estimates of 6-component mixture in Galaxy data
## =====
data(Galaxy, package="mixAK")
```

```
summary(Galaxy)

fit2 <- NMixEM(Galaxy, K = 6)
y <- seq(5, 40, length=300)
fy <- dMVNmixture(y, weight=fit2$weight, mean=fit2$mean,
                  Sigma=rep(fit2$Sigma, fit2$K))
hist(Galaxy, prob=TRUE, breaks=seq(5, 40, by=0.5),
     main="", xlab="Velocity (km/sec)", col="sandybrown")
lines(y, fy, col="darkblue", lwd=2)

## End(Not run)
```

---

 NMixMCMC

*MCMC estimation of (multivariate) normal mixtures with possibly censored data.*

---

### Description

This function runs MCMC for a model in which unknown density is specified as a normal mixture with either known or unknown number of components. With a prespecified number of components, MCMC is implemented through Gibbs sampling (see Diebolt and Robert, 1994) and dimension of the data can be arbitrary. With unknown number of components, currently only univariate case is implemented using the reversible jump MCMC (Richardson and Green, 1997).

Further, the data are allowed to be censored in which case additional Gibbs step is used within the MCMC algorithm

### Usage

```
NMixMCMC(y0, y1, censor, x_w, scale, prior,
         init, init2, RJMCMC,
         nMCMC = c(burn = 10, keep = 10, thin = 1, info = 10),
         PED, keep.chains = TRUE, onlyInit = FALSE, dens.zero = 1e-300,
         parallel = FALSE, cltype)
```

```
## S3 method for class 'NMixMCMC'
print(x, dic, ...)
```

```
## S3 method for class 'NMixMCMClist'
print(x, ped, dic, ...)
```

### Arguments

**y0** numeric vector of length  $n$  or  $n \times p$  matrix with observed data. It contains exactly observed, right-censored, left-censored data and lower limits for interval-censored data.

**y1** numeric vector of length  $n$  or  $n \times p$  matrix with upper limits for interval-censored data. Elements corresponding to exactly observed, right-censored or left-censored data are ignored and can be filled arbitrarily (by NA's) as well. It does not have to be supplied if there are no interval-censored data.

censor	<p>numeric vector of length <math>n</math> or <math>n \times p</math> matrix with censoring indicators. The following values indicate:</p> <p><b>0</b> right-censored observation,  <b>1</b> exactly observed value,  <b>2</b> left-censored observation,  <b>3</b> interval-censored observation.</p> <p>If it is not supplied then it is assumed that all values are exactly observed.</p>
x_w	<p>optional vector providing a categorical covariate that may influence the mixture weights. Internally, it is converted into a factor.</p> <p>Added in version 4.0 (03/2015).</p>
scale	<p>a list specifying how to scale the data before running MCMC. It should have two components:</p> <p><b>shift</b> a vector of length 1 or <math>p</math> specifying shift vector <math>m</math>,  <b>scale</b> a vector of length 1 or <math>p</math> specifying diagonal of the scaling matrix <math>S</math>.</p> <p>If there is no censoring, and argument <code>scale</code> is missing then the data are scaled to have zero mean and unit variances, i.e., <code>scale(y0)</code> is used for MCMC. In the case there is censoring and <code>scale</code> is missing, <code>scale\$shift</code> is taken to be a sample mean of <code>init\$y</code> and <code>scale\$scale</code> are sample standard deviations of columns of <code>init\$y</code>.</p> <p>If you do not wish to scale the data before running MCMC, specify <code>scale=list(shift=0, scale=1)</code>.</p>
prior	<p>a list with the parameters of the prior distribution. It should have the following components (for some of them, the program can assign default values and the user does not have to specify them if he/she wishes to use the defaults):</p> <p><b>priorK</b> a character string which specifies the type of the prior for <math>K</math> (the number of mixture components). It should have one of the following values:</p> <p>“fixed”  Number of mixture components is assumed to be fixed to <math>K_{max}</math>. This is a <b>default</b> value.</p> <p>“uniform”  A priori <math>K \sim \text{Unif}\{1, \dots, K_{max}\}</math>.</p> <p>“tpoisson”  A priori <math>K \sim \text{truncated-Poiss}(\lambda, K_{max})</math>.</p> <p><b>priormuQ</b> a character string which specifies the type of the prior for <math>\mu_1, \dots, \mu_{K_{max}}</math> (mixture means) and <math>Q_1, \dots, Q_{K_{max}}</math> (inverted mixture covariance matrices). It should have one of the following values:</p> <p>“independentC”  <math>\equiv</math> independent conjugate prior (this is a <b>default</b> value). That is, a priori</p> $(\mu_j, Q_j) \sim N(\xi_j, D_j) \times \text{Wishart}(\zeta, \Xi)$ <p>independently for <math>j = 1, \dots, K</math>, where normal means <math>\xi_1, \dots, \xi_K</math>, normal variances <math>D_1, \dots, D_K</math>, and Wishart degrees of freedom <math>\zeta</math> are specified further as xi, D, zeta components of the list prior.</p>

“naturalC”

≡ natural conjugate prior. That is, a priori

$$(\boldsymbol{\mu}_j, \mathbf{Q}_j) \sim \mathcal{N}(\boldsymbol{\xi}_j, c_j^{-1} \mathbf{Q}_j^{-1}) \times \text{Wishart}(\zeta, \boldsymbol{\Xi})$$

independently for  $j = 1, \dots, K$ , where normal means  $\boldsymbol{\xi}_1, \dots, \boldsymbol{\xi}_K$ , precisions  $c_1, \dots, c_K$ , and Wishart degrees of freedom  $\zeta$  are specified further as xi, ce, zeta components of the list prior.

For both, independent conjugate and natural conjugate prior, the Wishart scale matrix  $\boldsymbol{\Xi}$  is assumed to be diagonal with  $\gamma_1, \dots, \gamma_p$  on a diagonal. For  $\gamma_j^{-1}$  ( $j = 1, \dots, K$ ) additional gamma hyperprior  $G(g_j, h_j)$  is assumed. Values of  $g_1, \dots, g_p$  and  $h_1, \dots, h_p$  are further specified as g and h components of the prior list.

**Kmax** maximal number of mixture components  $K_{max}$ . It must **always be specified** by the user.

**lambda** parameter  $\lambda$  for the truncated Poisson prior on  $K$ . It must be positive and must **always be specified** if priorK is “tpoisson”.

**delta** parameter  $\delta$  for the Dirichlet prior on the mixture weights  $w_1, \dots, w_K$ . It must be positive. Its **default** value is 1.

**xi** a numeric value, vector or matrix which specifies  $\boldsymbol{\xi}_1, \dots, \boldsymbol{\xi}_{K_{max}}$  (prior means for the mixture means  $\boldsymbol{\mu}_1, \dots, \boldsymbol{\mu}_{K_{max}}$ ). **Default** value is a matrix  $K_{max} \times p$  with midpoints of columns of `init$y` in rows which follows Richardson and Green (1997).

If  $p = 1$  and `xi` =  $\xi$  is a single value then  $\xi_1 = \dots = \xi_{K_{max}} = \xi$ .

If  $p = 1$  and `xi` =  $\boldsymbol{\xi}$  is a vector of length  $K_{max}$  then the  $j$ -th element of `xi` gives  $\xi_j$  ( $j = 1, \dots, K_{max}$ ).

If  $p > 1$  and `xi` =  $\boldsymbol{\xi}$  is a vector of length  $p$  then  $\boldsymbol{\xi}_1 = \dots = \boldsymbol{\xi}_{K_{max}} = \boldsymbol{\xi}$ .

If  $p > 1$  and `xi` is a  $K_{max} \times p$  matrix then the  $j$ -th row of `xi` gives  $\boldsymbol{x}i_j$  ( $j = 1, \dots, K_{max}$ ).

**ce** a numeric value or vector which specifies prior precision parameters  $c_1, \dots, c_{K_{max}}$  for the mixture means  $\boldsymbol{\mu}_1, \dots, \boldsymbol{\mu}_{K_{max}}$  when `priormuQ` is “naturalC”. Its **default** value is a vector of ones which follows Cappe, Robert and Ryden (2003).

If `ce` =  $c$  is a single value then  $c_1 = \dots = c_{K_{max}} = c$ .

If `ce` =  $\boldsymbol{c}$  is a vector of length  $K_{max}$  then the  $j$ -th element of `ce` gives  $c_j$  ( $j = 1, \dots, K_{max}$ ).

**D** a numeric vector or matrix which specifies  $\mathbf{D}_1, \dots, \mathbf{D}_{K_{max}}$  (prior variances or covariance matrices of the mixture means  $\boldsymbol{\mu}_1, \dots, \boldsymbol{\mu}_{K_{max}}$  when `priormuQ` is “independentC”). Its **default** value is a diagonal matrix with squared ranges of each column of `init$y` on a diagonal.

If  $p = 1$  and  $D = d$  is a single value then  $d_1 = \dots = d_{K_{max}} = d$ .

If  $p = 1$  and  $D = \mathbf{d}$  is a vector of length  $K_{max}$  then the  $j$ -th element of  $D$  gives  $d_j$  ( $j = 1, \dots, K_{max}$ ).

If  $p > 1$  and  $D = \mathbf{D}$  is a  $p \times p$  matrix then  $D_1 = \dots = D_{K_{max}} = \mathbf{D}$ .

If  $p > 1$  and  $D$  is a  $(K_{max} \cdot p) \times p$  matrix then the first  $p$  rows of  $D$  give  $D_1$ , rows  $p + 1, \dots, 2p$  of  $D$  give  $D_2$  etc.

**zeta** degrees of freedom  $\zeta$  for the Wishart prior on the inverted mixture variances  $\mathbf{Q}_1, \dots, \mathbf{Q}_{K_{max}}$ . It must be higher than  $p - 1$ . Its **default** value is  $p + 1$ .

**g** a value or a vector of length  $p$  with the shape parameters  $g_1, \dots, g_p$  for the Gamma hyperpriors on  $\gamma_1, \dots, \gamma_p$ . It must be positive. Its **default** value is a vector  $(0.2, \dots, 0.2)'$ .

**h** a value or a vector of length  $p$  with the rate parameters  $h_1, \dots, h_p$  for the Gamma hyperpriors on  $\gamma_1, \dots, \gamma_p$ . It must be positive. Its **default** value is a vector containing  $10/R_l^2$ , where  $R_l$  is a range of the  $l$ -th column of `init$y`.

**init** a list with the initial values for the MCMC. All initials can be determined by the program if they are not specified. The list may have the following components:

**y** a numeric vector or matrix with the initial values for the latent censored observations.

**K** a numeric value with the initial value for the number of mixture components.

**w** a numeric vector with the initial values for the mixture weights.

**mu** a numeric vector or matrix with the initial values for the mixture means.

**Sigma** a numeric vector or matrix with the initial values for the mixture variances.

**Li** a numeric vector with the initial values for the Cholesky decomposition of the mixture inverse variances.

**gammaInv** a numeric vector with the initial values for the inverted components of the hyperparameter  $\gamma$ .

**r** a numeric vector with the initial values for the mixture allocations.

**init2** a list with the initial values for the second chain needed to estimate the penalized expected deviance of Plummer (2008). The list `init2` has the same structure as the list `init`. All initials in `init2` can be determined by the program (differently than the values in `init`) if they are not specified.

Ignored when PED is FALSE.

**RJMCMC** a list with the parameters needed to run reversible jump MCMC for mixtures with varying number of components. It does not have to be specified if the number of components is fixed. Most of the parameters can be determined by the program if they are not specified. The list may have the following components:

**Paction** probabilities (or proportional constants) which are used to choose an action of the sampler within each iteration of MCMC to update the mixture related parameters. Let `Paction` =  $(p_1, p_2, p_3)'$ . Then with probability  $p_1$  only steps assuming fixed  $k$  (number of mixture components) are

performed, with probability  $p_2$  split-combine move is proposed and with probability  $p_3$  birth-death move is proposed.

If not specified (default) then in each iteration of MCMC, all sampler actions are performed.

**Psplit** a numeric vector of length `prior$Kmax` giving conditional probabilities of the split move given  $k$  as opposite to the combine move.  
Default value is  $(1, 0.5, \dots, 0.5, 0)'$ .

**Pbirth** a numeric vector of length `prior$Kmax` giving conditional probabilities of the birth move given  $k$  as opposite to the death move.  
Default value is  $(1, 0.5, \dots, 0.5, 0)'$ .

**par.u1** a two component vector with parameters of the beta distribution used to generate an auxiliary value  $u_1$ .  
A default value is `par.u1 = (2, 2)'`, i.e.,  $u_1 \sim \text{Beta}(2, 2)$ .

**par.u2** a two component vector (for  $p = 1$ ) or a matrix (for  $p > 1$ ) with two columns with parameters of the distributions of the auxiliary values  $u_{2,1}, \dots, u_{2,p}$  in rows.  
A default value leads to  $u_{2,d} \sim \text{Unif}(-1, 1)$  ( $d = 1, \dots, p - 1$ ),  $u_{2,p} \sim \text{Beta}(1, 2p)$ .

**par.u3** a two component vector (for  $p = 1$ ) or a matrix (for  $p > 1$ ) with two columns with parameters of the distributions of the auxiliary values  $u_{3,1}, \dots, u_{3,p}$  in rows.  
A default value leads to  $u_{3,d} \sim \text{Unif}(0, 1)$  ( $d = 1, \dots, p - 1$ ),  $u_{3,p} \sim \text{Beta}(1, p)$ ,

nMCMC	numeric vector of length 4 giving parameters of the MCMC simulation. Its components may be named (ordering is then unimportant) as: <b>burn</b> length of the burn-in (after discarding the thinned values), can be equal to zero as well. <b>keep</b> length of the kept chains (after discarding the thinned values), must be positive. <b>thin</b> thinning interval, must be positive. <b>info</b> interval in which the progress information is printed on the screen. In total $(M_{burn} + M_{keep}) \cdot M_{thin}$ MCMC scans are performed.
PED	a logical value which indicates whether the penalized expected deviance (see Plummer, 2008 for more details) is to be computed (which requires two parallel chains). If not specified, PED is set to TRUE for models with fixed number of components and is set to FALSE for models with numbers of components estimated using RJ-MCMC.
keep.chains	logical. If FALSE, only summary statistics are returned in the resulting object. This might be useful in the model searching step to save some memory.
onlyInit	logical. If TRUE then the function only determines parameters of the prior distribution, initial values, values of <code>scale</code> and parameters for the reversible jump MCMC.
dens.zero	a small value used instead of zero when computing deviance related quantities.
x	an object of class NMixMCMC or NMixMCMClist to be printed.



<code>dic</code>	logical which indicates whether DIC should be printed. By default, DIC is printed only for models with a fixed number of mixture components.
<code>ped</code>	logical which indicates whether PED should be printed. By default, PED is printed only for models with a fixed number of mixture components.
<code>parallel</code>	a logical value which indicates whether parallel computation (based on a package <code>parallel</code> ) should be used when running two chains for the purpose of PED calculation
<code>cltype</code>	optional argument applicable if <code>parallel</code> is TRUE. If <code>cltype</code> is given, it is passed as the <code>type</code> argument into the call to <code>makeCluster</code> .
<code>...</code>	additional arguments passed to the default <code>print</code> method.

### Details

See accompanying paper (Komárek, 2009). In the rest of the helpfile, the same notation is used as in the paper, namely,  $n$  denotes the number of observations,  $p$  is dimension of the data,  $K$  is the number of mixture components,  $w_1, \dots, w_K$  are mixture weights,  $\mu_1, \dots, \mu_K$  are mixture means,  $\Sigma_1, \dots, \Sigma_K$  are mixture variance-covariance matrices,  $Q_1, \dots, Q_K$  are their inverses.

For the data  $\mathbf{y}_1, \dots, \mathbf{y}_n$  the following  $g_y(\mathbf{y})$  density is assumed

$$g_y(\mathbf{y}) = |\mathbf{S}|^{-1} \sum_{j=1}^K w_j \varphi(\mathbf{S}^{-1}(\mathbf{y} - \mathbf{m} | \mu_j, \Sigma_j)),$$

where  $\varphi(\cdot | \mu, \Sigma)$  denotes a density of the (multivariate) normal distribution with mean  $\mu$  and a variance-covariance matrix  $\Sigma$ . Finally,  $\mathbf{S}$  is a pre-specified diagonal scale matrix and  $\mathbf{m}$  is a pre-specified shift vector. Sometimes, by setting  $\mathbf{m}$  to sample means of components of  $\mathbf{y}$  and diagonal of  $\mathbf{S}$  to sample standard deviations of  $\mathbf{y}$  (considerable) improvement of the MCMC algorithm is achieved.

### Value

An object of class `NMixMCMC` or class `NMixMCMClist`. Object of class `NMixMCMC` is returned if PED is FALSE. Object of class `NMixMCMClist` is returned if PED is TRUE.

### Object of class NMixMCMC

Objects of class `NMixMCMC` have the following components:

- iter** index of the last iteration performed.
- nMCMC** used value of the argument `nMCMC`.
- dim** dimension  $p$  of the distribution of data
- nx\_w** number of levels of a factor covariate on mixture weights (equal to 1 if there were no covariates on mixture weights)
- prior** a list containing the used value of the argument `prior`.
- init** a list containing the used initial values for the MCMC (the first iteration of the burn-in).
- state.first** a list having the components labeled `y`, `K`, `w`, `mu`, `Li`, `Q`, `Sigma`, `gammaInv`, `r` containing the values of generic parameters at the first stored (after burn-in) iteration of the MCMC.

- state.last** a list having the components labeled y, K, w, mu, Li, Q, Sigma, gammaInv, r containing the last sampled values of generic parameters.
- RJMCMC** a list containing the used value of the argument RJMCMC.
- scale** a list containing the used value of the argument scale.
- freqK** frequency table of  $K$  based on the sampled chain.
- propK** posterior distribution of  $K$  based on the sampled chain.
- DIC** a data.frame having columns labeled DIC, pD, D.bar, D.in.bar containing values used to compute deviance information criterion (DIC). Currently only  $DIC_3$  of Celeux et al. (2006) is implemented.
- moves** a data.frame which summarizes the acceptance probabilities of different move types of the sampler.
- K** numeric vector with a chain for  $K$  (number of mixture components).
- w** numeric vector or matrix with a chain for  $w$  (mixture weights). It is a matrix with  $K$  columns when  $K$  is fixed. Otherwise, it is a vector with weights put sequentially after each other.
- mu** numeric vector or matrix with a chain for  $\mu$  (mixture means). It is a matrix with  $p \cdot K$  columns when  $K$  is fixed. Otherwise, it is a vector with means put sequentially after each other.
- Q** numeric vector or matrix with a chain for lower triangles of  $Q$  (mixture inverse variances). It is a matrix with  $\frac{p(p+1)}{2} \cdot K$  columns when  $K$  is fixed. Otherwise, it is a vector with lower triangles of  $Q$  matrices put sequentially after each other.
- Sigma** numeric vector or matrix with a chain for lower triangles of  $\Sigma$  (mixture variances). It is a matrix with  $\frac{p(p+1)}{2} \cdot K$  columns when  $K$  is fixed. Otherwise, it is a vector with lower triangles of  $\Sigma$  matrices put sequentially after each other.
- Li** numeric vector or matrix with a chain for lower triangles of Cholesky decompositions of  $Q$  matrices. It is a matrix with  $\frac{p(p+1)}{2} \cdot K$  columns when  $K$  is fixed. Otherwise, it is a vector with lower triangles put sequentially after each other.
- gammaInv** matrix with  $p$  columns with a chain for inverses of the hyperparameter  $\gamma$ .
- order** numeric vector or matrix with order indices of mixture components related to artificial identifiability constraint defined by a suitable re-labeling algorithm (by default, simple ordering of the first component of the mixture means is used).  
It is a matrix with  $K$  columns when  $K$  is fixed. Otherwise it is a vector with orders put sequentially after each other.
- rank** numeric vector or matrix with rank indices of mixture components. related to artificial identifiability constraint defined by a suitable re-labeling algorithm (by default, simple ordering of the first component of the mixture means is used).  
It is a matrix with  $K$  columns when  $K$  is fixed. Otherwise it is a vector with ranks put sequentially after each other.
- mixture** data.frame with columns labeled y.Mean.\*, y.SD.\*, y.Corr.\*, z.Mean.\*, z.SD.\*, z.Corr.\*.\* containing the chains for the means, standard deviations and correlations of the distribution of the original (y) and scaled (z) data based on a normal mixture at each iteration.
- deviance** data.frame with columns labels LogL0, LogL1, dev.complete, dev.observed containing the chains of quantities needed to compute DIC.
- pm.y** a data.frame with  $p$  columns with posterior means for (latent) values of observed data (useful when there is censoring).

**pm.z** a `data.frame` with  $p$  columns with posterior means for (latent) values of scaled observed data (useful when there is censoring).

**pm.indDev** a `data.frame` with columns labeled `LogL0`, `LogL1`, `dev.complete`, `dev.observed`, `pred.dens` containing posterior means of individual contributions to the deviance.

**pred.dens** a numeric vector with the predictive density of the data based on the MCMC sample evaluated at data points.

Note that when there is censoring, this is not exactly the predictive density as it is computed as the average of densities at each iteration evaluated at sampled values of latent observations at iterations.

**poster.comp.prob\_u** a matrix which is present in the output object if the number of mixture components in the distribution of random effects is fixed and equal to  $K$ . In that case, `poster.comp.prob_u` is a matrix with  $K$  columns and  $n$  rows with estimated posterior component probabilities – posterior means of the components of the underlying 0/1 allocation vector.

**WARNING:** By default, the labels of components are based on artificial identifiability constraints based on ordering of the mixture means in the first margin. Very often, such identifiability constraint is not satisfactory!

**poster.comp.prob\_b** a matrix which is present in the output object if the number of mixture components in the distribution of random effects is fixed and equal to  $K$ . In that case, `poster.comp.prob_b` is a matrix with  $K$  columns and  $n$  rows with estimated posterior component probabilities – posterior mean over model parameters.

**WARNING:** By default, the labels of components are based on artificial identifiability constraints based on ordering of the mixture means in the first margin. Very often, such identifiability constraint is not satisfactory!

**summ.y.Mean** Posterior summary statistics based on chains stored in `y.Mean.*` columns of the `data.frame` mixture.

**summ.y.SDCorr** Posterior summary statistics based on chains stored in `y.SD.*` and `y.Corr.*.*` columns of the `data.frame` mixture.

**summ.z.Mean** Posterior summary statistics based on chains stored in `z.Mean.*` columns of the `data.frame` mixture.

**summ.z.SDCorr** Posterior summary statistics based on chains stored in `z.SD.*` and `z.Corr.*.*` columns of the `data.frame` mixture.

**poster.mean.w** a numeric vector with posterior means of mixture weights after re-labeling. It is computed only if  $K$  is fixed and even then I am not convinced that these are useful posterior summary statistics (see label switching problem mentioned above). In any case, they should be used with care.

**poster.mean.mu** a matrix with posterior means of mixture means after re-labeling. It is computed only if  $K$  is fixed and even then I am not convinced that these are useful posterior summary statistics (see label switching problem mentioned above). In any case, they should be used with care.

**poster.mean.Q** a list with posterior means of mixture inverse variances after re-labeling. It is computed only if  $K$  is fixed and even then I am not convinced that these are useful posterior summary statistics (see label switching problem mentioned above). In any case, they should be used with care.

- poster.mean.Sigma** a list with posterior means of mixture variances after re-labeling. It is computed only if  $K$  is fixed and even then I am not convinced that these are useful posterior summary statistics (see label switching problem mentioned above). In any case, they should be used with care.
- poster.mean.Li** a list with posterior means of Cholesky decompositions of mixture inverse variances after re-labeling. It is computed only if  $K$  is fixed and even then I am not convinced that these are useful posterior summary statistics (see label switching problem mentioned above). In any case, they should be used with care.
- relabel** a list which specifies the algorithm used to re-label the MCMC output to compute order, rank, poster.comp.prob\_u, poster.comp.prob\_b, poster.mean.w, poster.mean.mu, poster.mean.Q, poster.mean.Sigma, poster.mean.Li.
- Cpar** a list with components useful to call underlying C++ functions (not interesting for ordinary users).

### Object of class NMixMCMClist

Object of class NMixMCMClist is the list having two components of class NMixMCMC representing two parallel chains and additionally the following components:

- PED** values of penalized expected deviance and related quantities. It is a vector with five components: D.expect = estimated expected deviance, where the estimate is based on two parallel chains; popt = estimated penalty, where the estimate is based on simple MCMC average based on two parallel chains; PED = estimated penalized expected deviance = D.expect + popt; wpopt = estimated penalty, where the estimate is based on weighted MCMC average (through importance sampling) based on two parallel chains; wPED = estimated penalized expected deviance = D.expect + wpopt.
- popt** contributions to the unweighted penalty from each observation.
- wpopt** contributions to the weighted penalty from each observation.
- inv.D** for each observation, number of iterations (in both chains), where the deviance was in fact equal to infinity (when the corresponding density was lower than dens.zero) and was not taken into account when computing D.expect.
- inv.popt** for each observation, number of iterations, where the penalty was in fact equal to infinity and was not taken into account when computing popt.
- inv.wpopt** for each observation, number of iterations, where the importance sampling weight was in fact equal to infinity and was not taken into account when computing wpopt.
- sumISw** for each observation, sum of importance sampling weights.

### Author(s)

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### References

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## See Also

[NMixPredDensMarg](#), [NMixPredDensJoint2](#).

## Examples

```
## Not run:
## See also additional material available in
## YOUR_R_DIR/library/mixAK/doc/
## or YOUR_R_DIR/site-library/mixAK/doc/
## - files Galaxy.R, Faithful.R, Tandmob.R and
## http://www.karlin.mff.cuni.cz/~komarek/software/mixAK/Galaxy.pdf
## http://www.karlin.mff.cuni.cz/~komarek/software/mixAK/Faithful.pdf
## http://www.karlin.mff.cuni.cz/~komarek/software/mixAK/Tandmob.pdf
##

## =====

## Simple analysis of Anderson's iris data
## =====
library("colorspace")

data(iris, package="datasets")
summary(iris)
VARS <- names(iris)[1:4]
#COLS <- rainbow_hcl(3, start = 60, end = 240)
COLS <- c("red", "darkblue", "darkgreen")
names(COLS) <- levels(iris[, "Species"])

### Prior distribution and the length of MCMC
Prior <- list(priorK = "fixed", Kmax = 3)
```

```

nMCMC <- c(burn=5000, keep=10000, thin=5, info=1000)

### Run MCMC
set.seed(20091230)
fit <- NMixMCMC(y0 = iris[, VARS], prior = Prior, nMCMC = nMCMC)

### Basic posterior summary
print(fit)

### Univariate marginal posterior predictive densities
### based on chain #1
pdens1 <- NMixPredDensMarg(fit[[1]], lgrid=150)
plot(pdens1)
plot(pdens1, main=VARS, xlab=VARS)

### Bivariate (for each pair of margins) predictive densities
### based on chain #1
pdens2a <- NMixPredDensJoint2(fit[[1]])
plot(pdens2a)

plot(pdens2a, xylab=VARS)
plot(pdens2a, xylab=VARS, contour=TRUE)

### Determine the grid to compute bivariate densities
grid <- list(Sepal.Length=seq(3.5, 8.5, length=75),
            Sepal.Width=seq(1.8, 4.5, length=75),
            Petal.Length=seq(0, 7, length=75),
            Petal.Width=seq(-0.2, 3, length=75))
pdens2b <- NMixPredDensJoint2(fit[[1]], grid=grid)
plot(pdens2b, xylab=VARS)

### Plot with contours
ICOL <- rev(heat_hcl(20, c=c(80, 30), l=c(30, 90), power=c(1/5, 2)))
oldPar <- par(mfrow=c(2, 3), bty="n")
for (i in 1:3){
  for (j in (i+1):4){
    NAME <- paste(i, "-", j, sep="")
    MAIN <- paste(VARS[i], "x", VARS[j])
    image(pdens2b$x[[i]], pdens2b$x[[j]], pdens2b$dens[[NAME]], col=ICOL,
          xlab=VARS[i], ylab=VARS[j], main=MAIN)
    contour(pdens2b$x[[i]], pdens2b$x[[j]], pdens2b$dens[[NAME]], add=TRUE, col="brown4")
  }
}

### Plot with data
for (i in 1:3){
  for (j in (i+1):4){
    NAME <- paste(i, "-", j, sep="")
    MAIN <- paste(VARS[i], "x", VARS[j])
    image(pdens2b$x[[i]], pdens2b$x[[j]], pdens2b$dens[[NAME]], col=ICOL,
          xlab=VARS[i], ylab=VARS[j], main=MAIN)
    for (spec in levels(iris[, "Species"])){
      Data <- subset(iris, Species==spec)

```

```

        points(Data[,i], Data[,j], pch=16, col=COLS[spec])
      }
    }
  }

  ### Set the graphical parameters back to their original values
  par(oldPar)

  ### Clustering based on posterior summary statistics of component allocations
  ### or on the posterior distribution of component allocations
  ### (these are two equivalent estimators of probabilities of belonging
  ### to each mixture components for each observation)
  p1 <- fit[[1]]$poster.comp.prob_u
  p2 <- fit[[1]]$poster.comp.prob_b

  ### Clustering based on posterior summary statistics of mixture weight, means, variances
  p3 <- NMixPlugDA(fit[[1]], iris[, VARS])
  p3 <- p3[, paste("prob", 1:3, sep="")]

  ### Observations from "setosa" species (all would be allocated in component 1)
  apply(p1[1:50,], 2, quantile, prob=seq(0, 1, by=0.1))
  apply(p2[1:50,], 2, quantile, prob=seq(0, 1, by=0.1))
  apply(p3[1:50,], 2, quantile, prob=seq(0, 1, by=0.1))

  ### Observations from "versicolor" species (almost all would be allocated in component 2)
  apply(p1[51:100,], 2, quantile, prob=seq(0, 1, by=0.1))
  apply(p2[51:100,], 2, quantile, prob=seq(0, 1, by=0.1))
  apply(p3[51:100,], 2, quantile, prob=seq(0, 1, by=0.1))

  ### Observations from "virginica" species (all would be allocated in component 3)
  apply(p1[101:150,], 2, quantile, prob=seq(0, 1, by=0.1))
  apply(p2[101:150,], 2, quantile, prob=seq(0, 1, by=0.1))
  apply(p3[101:150,], 2, quantile, prob=seq(0, 1, by=0.1))

  ## End(Not run)

```

---

NMmixPlugCondDensJoint2

*Pairwise bivariate conditional densities: plug-in estimate*

---

## Description

This function serves as an inference tool for the MCMC output obtained using the function [NMixMCMC](#). It computes estimates of pairwise bivariate conditional densities (given one margin) obtained by using posterior summary statistics (e.g., posterior means) of mixture weights, means and variances (plug-in estimate).

## Usage

```
NMmixPlugCondDensJoint2(x, ...)
```

```
## Default S3 method:
NMixPlugCondDensJoint2(x, icond, scale, w, mu, Sigma, ...)

## S3 method for class 'NMixMCMC'
NMixPlugCondDensJoint2(x, icond, grid, lgrid=50, scaled=FALSE, ...)

## S3 method for class 'GLMM_MCMC'
NMixPlugCondDensJoint2(x, icond, grid, lgrid=50, scaled=FALSE, ...)
```

### Arguments

<code>x</code>	an object of class <code>NMixMCMC</code> for <code>NMixPlugCondDensJoint2.NMixMCMC</code> function. An object of class <code>GLMM_MCMC</code> for <code>NMixPlugCondDensJoint2.GLMM_MCMC</code> function. A list with the grid values (see below) for <code>NMixPlugCondDensJoint2.default</code> function.
<code>icond</code>	index of the margin by which we want to condition
<code>scale</code>	a two component list giving the shift and the scale. If not given, shift is equal to zero and scale is equal to one.
<code>w</code>	a numeric vector with posterior summary statistics for the mixture weights. The length of this vector determines the number of mixture components.
<code>mu</code>	a matrix with posterior summary statistics for mixture means in rows. That is, <code>mu</code> has $K$ rows and $p$ columns, where $K$ denotes the number of mixture components and $p$ is dimension of the mixture distribution.
<code>Sigma</code>	a list with posterior summary statistics for mixture covariance matrices.
<code>grid</code>	a list with the grid values for each margin in which the density should be evaluated. The value of <code>grid[[icond]]</code> determines the values by which we condition. If <code>grid</code> is not specified, it is created automatically using the information from the posterior summary statistics stored in <code>x</code> .
<code>lgrid</code>	a length of the grid used to create the <code>grid</code> if that is not specified.
<code>scaled</code>	if <code>TRUE</code> , the density of shifted and scaled data is summarized. The shift and scale vector are taken from the <code>scale</code> component of the object <code>x</code> .
<code>...</code>	optional additional arguments.

### Value

An object of class `NMixPlugCondDensJoint2` which has the following components:

<code>x</code>	a list with the grid values for each margin. The components of the list are named <code>x1</code> , <code>...</code> or take names from <code>grid</code> argument.
<code>icond</code>	index of the margin by which we condition.



`dens` a list with the computed conditional densities for each value of `x[[icond]]`. Each `dens[[j]]` is again a list with conditional densities for each pair of margins given margin `icond` equal to `x[[icond]][j]`. The value of `dens[[j]][[i-k]]` gives values of conditional density of the (i,k)-th margins given margin `icond` equal to `x[[icond]][j]`.

There is also a `plot` method implemented for the resulting object.

### Author(s)

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

### See Also

[plot.NMixPlugCondDensJoint2](#), [NMixMCMC](#), [GLMM\\_MCMC](#), [NMixPredCondDensJoint2](#).

---

NMixPlugCondDensMarg *Univariate conditional densities: plug-in estimate*

---

### Description

This function serves as an inference tool for the MCMC output obtained using the function [NMixMCMC](#). It computes estimates of univariate conditional densities obtained by using posterior summary statistics (e.g., posterior means) of mixture weights, means and variances (plug-in estimate).

### Usage

```
NMixPlugCondDensMarg(x, ...)

## Default S3 method:
NMixPlugCondDensMarg(x, icond, scale, w, mu, Sigma, ...)

## S3 method for class 'NMixMCMC'
NMixPlugCondDensMarg(x, icond, grid, lgrid=50, scaled=FALSE, ...)

## S3 method for class 'GLMM_MCMC'
NMixPlugCondDensMarg(x, icond, grid, lgrid=50, scaled=FALSE, ...)
```

### Arguments

`x` an object of class `NMixMCMC` for `NMixPlugCondDensMarg.NMixMCMC` function. An object of class `GLMM_MCMC` for `NMixPlugCondDensMarg.GLMM_MCMC` function.  
A list with the grid values (see below) for `NMixPlugCondDensMarg.default` function.

`icond` index of the margin by which we want to condition

scale	a two component list giving the shift and the scale. If not given, shift is equal to zero and scale is equal to one.
w	a numeric vector with posterior summary statistics for the mixture weights. The length of this vector determines the number of mixture components.
mu	a matrix with posterior summary statistics for mixture means in rows. That is, mu has $K$ rows and $p$ columns, where $K$ denotes the number of mixture components and $p$ is dimension of the mixture distribution.
Sigma	a list with posterior summary statistics for mixture covariance matrices.
grid	a list with the grid values for each margin in which the density should be evaluated. The value of <code>grid[[icond]]</code> determines the values by which we condition.  If <code>grid</code> is not specified, it is created automatically using the information from the posterior summary statistics stored in <code>x</code> .
lgrid	a length of the grid used to create the <code>grid</code> if that is not specified.
scaled	if TRUE, the density of shifted and scaled data is summarized. The shift and scale vector are taken from the <code>scale</code> component of the object <code>x</code> .
...	optional additional arguments.

### Value

An object of class `NMixPlugCondDensMarg` which has the following components:

x	a list with the grid values for each margin. The components of the list are named <code>x1</code> , ... or take names from <code>grid</code> argument.
icond	index of the margin by which we condition.
dens	a list with the computed conditional densities for each value of <code>x[[icond]]</code> . Each <code>dens[[j]]</code> is again a list with conditional densities for each margin given margin <code>icond</code> equal to <code>x[[icond]][j]</code> . The value of <code>dens[[j]][[imargin]]</code> gives a value of a marginal density of the <code>imargin</code> -th margin at <code>x[[icond]][j]</code> .

There is also a `plot` method implemented for the resulting object.

### Author(s)

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

### See Also

[plot.NMixPlugCondDensMarg](#), [NMixMCMC](#), [GLMM\\_MCMC](#), [NMixPredCondDensMarg](#).

---

NMixPlugDA	<i>Discriminant analysis based on plug-in estimates from the mixture model</i>
------------	--

---

### Description

It performs discriminant analysis based on posterior summary for (re-labeled) mixture components in a model with fixed number of components fitted with [NMixMCMC](#) function.

### Usage

```
NMixPlugDA(object, y)
```

### Arguments

object	an object of class NMixMCMC
y	vector, matrix or data frame with observations to be clustered

### Value

A data.frame with columns labeled prob1,..., probp giving plug-in estimates of probabilities of belonging to each component and a column labeled component giving the index of the component with the highest component probability.

### Author(s)

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

### See Also

[NMixMCMC](#), [NMixPredDA](#).

---

NMixPlugDensJoint2	<i>Pairwise bivariate densities: plug-in estimate</i>
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---

### Description

This function serves as an inference tool for the MCMC output obtained using the function [NMixMCMC](#). It computes marginal (pairwise bivariate) plug-in densities obtained by using posterior summary statistics (e.g., posterior means) of mixture weights, means and variances.

**Usage**

```

NMixPlugDensJoint2(x, ...)

## Default S3 method:
NMixPlugDensJoint2(x, scale, w, mu, Sigma, ...)

## S3 method for class 'NMixMCMC'
NMixPlugDensJoint2(x, grid, lgrid=50, scaled=FALSE, ...)

## S3 method for class 'GLMM_MCMC'
NMixPlugDensJoint2(x, grid, lgrid=50, scaled=FALSE, ...)

```

**Arguments**

<code>x</code>	an object of class <code>NMixMCMC</code> for <code>NMixPlugDensJoint2.NMixMCMC</code> function. An object of class <code>GLMM_MCMC</code> for <code>NMixPlugDensJoint2.GLMM_MCMC</code> function. A list with the grid values (see below) for <code>NMixPlugDensJoint2.default</code> function.
<code>scale</code>	a two component list giving the shift and the scale. If not given, shift is equal to zero and scale is equal to one.
<code>w</code>	a numeric vector with posterior summary statistics for the mixture weights. The length of this vector determines the number of mixture components.
<code>mu</code>	a matrix with posterior summary statistics for mixture means in rows. That is, $\mu$ has $K$ rows and $p$ columns, where $K$ denotes the number of mixture components and $p$ is dimension of the mixture distribution.
<code>Sigma</code>	a list with posterior summary statistics for for mixture covariance matrices.
<code>grid</code>	a list with the grid values for each margin in which the density should be evaluated.  If <code>grid</code> is not specified, it is created automatically using the information from the posterior summary statistics stored in <code>x</code> .
<code>lgrid</code>	a length of the grid used to create the <code>grid</code> if that is not specified.
<code>scaled</code>	if <code>TRUE</code> , the density of shifted and scaled data is summarized. The shift and scale vector are taken from the <code>scale</code> component of the object <code>x</code> .
<code>...</code>	optional additional arguments.

**Value**

An object of class `NMixPlugDensJoint2` which has the following components:

<code>x</code>	a list with the grid values for each margin. The components of the list are named <code>x1, ...</code> or take names from <code>grid</code> argument.
<code>dens</code>	a list with the computed densities for each pair of margins. The components of the list are named <code>1-2, 1-3, ...</code> , i.e., <code>dens[[1]]=dens[["1-2"]]</code> is the pairwise predictive density for margins 1 and 2, etc. Each component of the list is a matrix in such a form that it can be directly passed together with the proper components of <code>x</code> to the plotting functions like <code>contour</code> or <code>image</code> .

There is also a `plot` method implemented for the resulting object.

### Author(s)

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

### See Also

[plot.NMixPlugDensJoint2](#), [NMixMCMC](#), [GLMM\\_MCMC](#), [NMixPredDensJoint2](#).

---

NMixPlugDensMarg	<i>Marginal (univariate) densities: plug-in estimate</i>
------------------	--

---

### Description

This function serves as an inference tool for the MCMC output obtained using the function [NMixMCMC](#). It computes marginal (univariate) plug-in densities obtained by using posterior summary statistics (e.g., posterior means) of mixture weights, means and variances.

### Usage

```
NMixPlugDensMarg(x, ...)

## Default S3 method:
NMixPlugDensMarg(x, scale, w, mu, Sigma, ...)

## S3 method for class 'NMixMCMC'
NMixPlugDensMarg(x, grid, lgrid=500, scaled=FALSE, ...)

## S3 method for class 'GLMM_MCMC'
NMixPlugDensMarg(x, grid, lgrid=500, scaled=FALSE, ...)
```

### Arguments

<code>x</code>	a list with the grid values (see below) for <code>NMixPlugDensMarg.default</code> function. An object of class <code>NMixMCMC</code> for <code>NMixPlugDensMarg.NMixMCMC</code> function. An object of class <code>GLMM_MCMC</code> for <code>NMixPlugDensMarg.GLMM_MCMC</code> function.
<code>scale</code>	a two component list giving the shift and the scale. If not given, shift is equal to zero and scale is equal to one.
<code>w</code>	a numeric vector with posterior summary statistics for the mixture weights. The length of this vector determines the number of mixture components.
<code>mu</code>	a matrix with posterior summary statistics for mixture means in rows. That is, <code>mu</code> has $K$ rows and $p$ columns, where $K$ denotes the number of mixture components and $p$ is dimension of the mixture distribution.
<code>Sigma</code>	a list with posterior summary statistics for mixture covariance matrices.

grid	a list with the grid values for each margin in which the density should be evaluated. If grid is not specified, it is created automatically using the information from the posterior summary statistics stored in x.
lgrid	a length of the grid used to create the grid if that is not specified.
scaled	if TRUE, the density of shifted and scaled data is summarized. The shift and scale vector are taken from the scale component of the object x.
...	optional additional arguments.

**Value**

An object of class `NMixPlugDensMarg` which has the following components:

x	a list with the grid values for each margin. The components of the list are named x1, ... or take names from grid argument.
dens	a list with the computed densities for each margin. The components of the list are named 1, ..., i.e., <code>dens[[1]]=dens[["1"]]</code> is the predictive density for margin 1 etc.

There is also a `plot` method implemented for the resulting object.

**Author(s)**

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

**See Also**

[plot.NMixPlugDensMarg](#), [NMixMCMC](#), [GLMM\\_MCMC](#), [NMixPredDensMarg](#).

---

NMixPredCDFMarg	<i>Marginal (univariate) predictive cumulative distribution function</i>
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---

**Description**

This function serves as an inference tool for the MCMC output obtained using the function [NMixMCMC](#). It computes estimated posterior predictive cumulative distribution function for each margin.

**Usage**

```
NMixPredCDFMarg(x, ...)

## Default S3 method:
NMixPredCDFMarg(x, scale, K, w, mu, Li, Krandom=TRUE, ...)

## S3 method for class 'NMixMCMC'
NMixPredCDFMarg(x, grid, lgrid=500, scaled=FALSE, ...)

## S3 method for class 'GLMM_MCMC'
NMixPredCDFMarg(x, grid, lgrid=500, scaled=FALSE, ...)
```

**Arguments**

x	an object of class NMixMCMC for NMixPredCDFMarg.NMixMCMC function. An object of class GLMM_MCMC for NMixPredCDFMarg.GLMM_MCMC function.
scale	A list with the grid values (see below) for NMixPredCDFMarg.default function. a two component list giving the shift and the scale.
K	either a number (when Krandom=FALSE) or a numeric vector with the chain for the number of mixture components.
w	a numeric vector with the chain for the mixture weights.
mu	a numeric vector with the chain for the mixture means.
Li	a numeric vector with the chain for the mixture inverse variances (lower triangles only).
Krandom	a logical value which indicates whether the number of mixture components changes from one iteration to another.
grid	a numeric vector or a list with the grid values in which the predictive CDF should be evaluated. If x\$dim is 1 then grid may be a numeric vector. If x\$dim is higher than then grid must be a list with numeric vectors as components giving the grids for each margin. If grid is not specified, it is created automatically using the information from the posterior summary statistics stored in x.
lgrid	a length of the grid used to create the grid if that is not specified.
scaled	if TRUE, the CDF of shifted and scaled data is summarized. The shift and scale vector are taken from the scale component of the object x.
...	optional additional arguments.

**Value**

An object of class NMixPredCDFMarg which has the following components:

x	a list with the grid values for each margin. The components of the list are named x1, ... or take names from grid argument.
freqK	frequency table for the values of $K$ (numbers of mixture components) in the MCMC chain.
propK	proportions derived from freqK.
MCMC.length	the length of the MCMC used to compute the predictive cdf's.
cdf	a list with the computed predictive CDF's for each margin. The components of the list are named 1, ..., i.e., $\text{cdf}[[1]] = \text{cdf}[["1"]]$ is the predictive cdf for margin 1 etc.
cdfK	a list with the computed predictive CDF's for each margin, conditioned further by $K$ . The components of the list are named 1, .... That is, $\text{cdf}[[1]][[1]] = \text{cdf}[["1"]][[1]]$ is the predictive CDF for margin 1 conditioned by $K = 1$ , $\text{cdf}[[1]][[2]] = \text{cdf}[["1"]][[2]]$ is the predictive CDF for margin 1 conditioned by $K = 2$ etc. Note that cdfK provides some additional information only when Krandom = TRUE or when x results from the <a href="#">NMixMCMC</a> call to the reversible jump MCMC.

There is also a `plot` method implemented for the resulting object.

### Author(s)

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

### References

Komárek, A. (2009). A new R package for Bayesian estimation of multivariate normal mixtures allowing for selection of the number of components and interval-censored data. *Computational Statistics and Data Analysis*, **53**(12), 3932–3947.

### See Also

[plot.NMixPredCDFMarg](#), [NMixMCMC](#), [GLMM\\_MCMC](#).

---

NMixPredCondCDFMarg     *Univariate conditional predictive cumulative distribution function*

---

### Description

This function serves as an inference tool for the MCMC output obtained using the function [NMixMCMC](#). It computes (posterior predictive) estimates of univariate conditional cumulative distribution functions.

### Usage

```
NMixPredCondCDFMarg(x, ...)

## Default S3 method:
NMixPredCondCDFMarg(x, icond, prob, scale, K, w, mu, Li, Krandom=FALSE, ...)

## S3 method for class 'NMixMCMC'
NMixPredCondCDFMarg(x, icond, prob, grid, lgrid=50, scaled=FALSE, ...)

## S3 method for class 'GLMM_MCMC'
NMixPredCondCDFMarg(x, icond, prob, grid, lgrid=50, scaled=FALSE, ...)
```

### Arguments

<code>x</code>	an object of class <code>NMixMCMC</code> for <code>NMixPredCondCDFMarg.NMixMCMC</code> function. An object of class <code>GLMM_MCMC</code> for <code>NMixPredCondCDFMarg.GLMM_MCMC</code> function. A list with the grid values (see below) for <code>NMixPredCondCDFMarg.default</code> function.
<code>icond</code>	index of the margin by which we want to condition



prob	a numeric vector. If given then also the posterior pointwise quantiles of the conditional cdf's are computed for probabilities given by prob. These can be used to draw pointwise credible intervals.
scale	a two component list giving the shift and the scale. If not given, shift is equal to zero and scale is equal to one.
K	either a number (when Krandom=FALSE) or a numeric vector with the chain for the number of mixture components.
w	a numeric vector with the chain for the mixture weights.
mu	a numeric vector with the chain for the mixture means.
Li	a numeric vector with the chain for the mixture inverse variances (lower triangles only).
Krandom	a logical value which indicates whether the number of mixture components changes from one iteration to another.
grid	a list with the grid values for each margin in which the cdf should be evaluated. The value of grid[[icond]] determines the values by which we condition. If grid is not specified, it is created automatically using the information from the posterior summary statistics stored in x.
lgrid	a length of the grid used to create the grid if that is not specified.
scaled	if TRUE, the cdf of shifted and scaled data is summarized. The shift and scale vector are taken from the scale component of the object x.
...	optional additional arguments.

### Value

An object of class NMixPredCondCDFMarg which has the following components:

x	a list with the grid values for each margin. The components of the list are named x1, ... or take names from grid argument.
icond	index of the margin by which we condition.
cdf	a list with the computed conditional cdf's for each value of x[[icond]]. Each cdf[[j]] is again a list with conditional cdf's for each margin given margin icond equal to x[[icond]][j]. The value of cdf[[j]][[imargin]] gives a value of a marginal cdf of the imargin-th margin at x[[icond]][j].
prob	a value of the argument prob.
‘‘qXX%’’	if prob is given then there is one additional component named ‘‘qXX%’’, e.g., ‘‘q50%’’ for each value of prob which has the same structure as the component cdf and keeps computed posterior pointwise quantiles.

There is also a plot method implemented for the resulting object.

### Author(s)

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

### See Also

[plot.NMixPredCondCDFMarg](#), [NMixMCMC](#), [GLMM\\_MCMC](#).

---

 NMixPredCondDensJoint2

*Pairwise bivariate conditional predictive densities*


---

## Description

This function serves as an inference tool for the MCMC output obtained using the function [NMixMCMC](#). It computes (posterior predictive) estimates of pairwise bivariate conditional densities (given one margin).

## Usage

```

NMixPredCondDensJoint2(x, ...)

## Default S3 method:
NMixPredCondDensJoint2(x, icond, scale, K, w, mu, Li, Krandom=FALSE, ...)

## S3 method for class 'NMixMCMC'
NMixPredCondDensJoint2(x, icond, grid, lgrid=50, scaled=FALSE, ...)

## S3 method for class 'GLMM_MCMC'
NMixPredCondDensJoint2(x, icond, grid, lgrid=50, scaled=FALSE, ...)

```

## Arguments

x	an object of class NMixMCMC for NMixPredCondDensJoint2.NMmixMCMC function. An object of class GLMM_MCMC for NMixPredCondDensJoint2.GLMM_MCMC function. A list with the grid values (see below) for NMixPredCondDensJoint2.default function.
icond	index of the margin by which we want to condition
scale	a two component list giving the shift and the scale. If not given, shift is equal to zero and scale is equal to one.
K	either a number (when Krandom=FALSE) or a numeric vector with the chain for the number of mixture components.
w	a numeric vector with the chain for the mixture weights.
mu	a numeric vector with the chain for the mixture means.
Li	a numeric vector with the chain for the mixture inverse variances (lower triangles only).
Krandom	a logical value which indicates whether the number of mixture components changes from one iteration to another.
grid	a list with the grid values for each margin in which the density should be evaluated. The value of grid[[icond]] determines the values by which we condition.

	If <code>grid</code> is not specified, it is created automatically using the information from the posterior summary statistics stored in <code>x</code> .
<code>lgrid</code>	a length of the grid used to create the <code>grid</code> if that is not specified.
<code>scaled</code>	if TRUE, the density of shifted and scaled data is summarized. The shift and scale vector are taken from the scale component of the object <code>x</code> .
<code>...</code>	optional additional arguments.

**Value**

An object of class `NMixPredCondDensJoint2` which has the following components:

<code>x</code>	a list with the <code>grid</code> values for each margin. The components of the list are named <code>x1, ...</code> or take names from <code>grid</code> argument.
<code>icond</code>	index of the margin by which we condition.
<code>dens</code>	a list with the computed conditional densities for each value of <code>x[[icond]]</code> . Each <code>dens[[j]]</code> is again a list with conditional densities for each pair of margins given margin <code>icond</code> equal to <code>x[[icond]][j]</code> . The value of <code>dens[[j]][[i-k]]</code> gives values of conditional density of the (i,k)-th margins given margin <code>icond</code> equal to <code>x[[icond]][j]</code> .

There is also a `plot` method implemented for the resulting object.

**Author(s)**

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

**See Also**

[plot.NMixPredCondDensJoint2](#), [NMixMCMC](#), [GLMM\\_MCMC](#).

---

`NMixPredCondDensMarg` *Univariate conditional predictive density*

---

**Description**

This function serves as an inference tool for the MCMC output obtained using the function [NMixMCMC](#). It computes (posterior predictive) estimates of univariate conditional densities.

**Usage**

```
NMixPredCondDensMarg(x, ...)

## Default S3 method:
NMixPredCondDensMarg(x, icond, prob, scale, K, w, mu, Li, Krandom=FALSE, ...)

## S3 method for class 'NMixMCMC'
NMixPredCondDensMarg(x, icond, prob, grid, lgrid=50, scaled=FALSE, ...)
```

```
## S3 method for class 'GLMM_MCMC'
NMixPredCondDensMarg(x, icond, prob, grid, lgrid=50, scaled=FALSE, ...)
```

### Arguments

x	an object of class NMixMCMC for NMixPredCondDensMarg.NMCMC function. An object of class GLMM_MCMC for NMixPredCondDensMarg.GLMM_MCMC function. A list with the grid values (see below) for NMixPredCondDensMarg.default function.
icond	index of the margin by which we want to condition
prob	a numeric vector. If given then also the posterior pointwise quantiles of the conditional densities are computed for probabilities given by prob. These can be used to draw pointwise credible intervals.
scale	a two component list giving the shift and the scale. If not given, shift is equal to zero and scale is equal to one.
K	either a number (when Krandom=FALSE) or a numeric vector with the chain for the number of mixture components.
w	a numeric vector with the chain for the mixture weights.
mu	a numeric vector with the chain for the mixture means.
Li	a numeric vector with the chain for the mixture inverse variances (lower triangles only).
Krandom	a logical value which indicates whether the number of mixture components changes from one iteration to another.
grid	a list with the grid values for each margin in which the density should be evaluated. The value of grid[[icond]] determines the values by which we condition. If grid is not specified, it is created automatically using the information from the posterior summary statistics stored in x.
lgrid	a length of the grid used to create the grid if that is not specified.
scaled	if TRUE, the density of shifted and scaled data is summarized. The shift and scale vector are taken from the scale component of the object x.
...	optional additional arguments.

### Value

An object of class NMixPredCondDensMarg which has the following components:

x	a list with the grid values for each margin. The components of the list are named x1, ... or take names from grid argument.
icond	index of the margin by which we condition.
dens	a list with the computed conditional densities for each value of x[[icond]]. Each dens[[j]] is again a list with conditional densities for each margin given margin icond equal to x[[icond]][j]. The value of dens[[j]][[imargin]] gives a value of a marginal density of the imargin-th margin at x[[icond]][j].

prob a value of the argument prob.  
 ‘ ‘qXX%’ ’ if prob is given then there is one additional component named “qXX%”, e.g., “q50%” for each value of prob which has the same structure as the component dens and keeps computed posterior pointwise quantiles.

There is also a `plot` method implemented for the resulting object.

### Author(s)

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

### See Also

[plot.NMixPredCondDensMarg](#), [NMixMCMC](#), [GLMM\\_MCMC](#).

---

NMixPredDA

*Discriminant analysis based on MCMC output from the mixture model*

---

### Description

It performs discriminant analysis based on sampled (re-labeled) MCMC chains from the mixture model fitted with [NMixMCMC](#) function. Observations to be discriminated may be censored.

Discrimination is based on posterior predictive probabilities of belonging to (re-labeled) mixture components.

### Usage

```
NMixPredDA(object, y0, y1, censor, inity, info)
```

### Arguments

object an object of class `NMixMCMC`  
 y0 vector, matrix or data frame with observations (or limits of censored-observations) to be clustered. See [NMixMCMC](#) for details.  
 If y0 is not given then the function discriminates original observations used to generate MCMC sample stored in object.  
 y1 vector, matrix or data frame with upper limits of interval-censored observations (if there are any). See [NMixMCMC](#) for details.  
 censor vector, matrix or data frame with censoring indicators (if there are any censored observations). See [NMixMCMC](#) for details.  
 inity optional vector, matrix or data frame with initial values of censored observations (if there are any censored observations)  
 info number which specifies frequency used to re-display the iteration counter during the computation.

**Value**

A data.frame with columns labeled prob1,..., probp giving posterior predictive probabilities of belonging to each component and a column labeled component giving the index of the component with the highest component probability.

**Author(s)**

Arnošt Komárek <arnost.komarek[AT]mf.f.cuni.cz>

**See Also**

[NMixMCMC](#), [NMixPlugDA](#).

---

NMixPredDensJoint2      *Pairwise bivariate predictive density*

---

**Description**

This function serves as an inference tool for the MCMC output obtained using the function [NMixMCMC](#). It computes estimated posterior predictive densities for each pair of margins.

**Usage**

```

NMixPredDensJoint2(x, ...)

## Default S3 method:
NMixPredDensJoint2(x, scale, K, w, mu, Li, Krandom=TRUE, ...)

## S3 method for class 'NMixMCMC'
NMixPredDensJoint2(x, grid, lgrid=50, scaled=FALSE, ...)

## S3 method for class 'GLMM_MCMC'
NMixPredDensJoint2(x, grid, lgrid=50, scaled=FALSE, ...)

```

**Arguments**

x	an object of class NMixMCMC for NMixPredDensJoint2.NMixMCMC function. an object of class GLMM_MCMC for NMixPredDensJoint2.GLMM_MCMC function. A list with the grid values (see below) for NMixPredDensJoint2.default function.
scale	a two component list giving the shift and the scale. If not given, shift is equal to zero and scale is equal to one.
K	either a number (when Krandom=FALSE) or a numeric vector with the chain for the number of mixture components.
w	a numeric vector with the chain for the mixture weights.

<code>mu</code>	a numeric vector with the chain for the mixture means.
<code>Li</code>	a numeric vector with the chain for the mixture inverse variances (lower triangles only).
<code>Krandom</code>	a logical value which indicates whether the number of mixture components changes from one iteration to another.
<code>grid</code>	a list with the grid values for each margin in which the predictive density should be evaluated. If <code>grid</code> is not specified, it is created automatically using the information from the posterior summary statistics stored in <code>x</code> .
<code>lgrid</code>	a length of the grid used to create the <code>grid</code> if that is not specified.
<code>scaled</code>	if TRUE, the density of shifted and scaled data is summarized. The shift and scale vector are taken from the scale component of the object <code>x</code> .
<code>...</code>	optional additional arguments.

### Value

An object of class `NMixPredDensJoint2` which has the following components:

<code>x</code>	a list with the grid values for each margin. The components of the list are named <code>x1, ...</code> or take names from <code>grid</code> argument.
<code>freqK</code>	frequency table for the values of $K$ (numbers of mixture components) in the MCMC chain.
<code>propK</code>	proportions derived from <code>freqK</code> .
<code>MCMC.length</code>	the length of the MCMC used to compute the predictive densities.
<code>dens</code>	a list with the computed predictive densities for each pair of margins. The components of the list are named <code>1-2, 1-3, ...</code> , i.e., <code>dens[[1]] = dens[["1-2"]]</code> is the pairwise predictive density for margins 1 and 2, etc. Each component of the list is a matrix in such a form that it can be directly passed together with the proper components of <code>x</code> to the plotting functions like <code>contour</code> or <code>image</code> .
<code>densK</code>	a list with the computed predictive densities for each margin, conditioned further by $K$ . The components of the list are named <code>1-2, 1-3, ...</code> . That is, <code>dens[[1]][[1]] = dens[["1-2"]][[1]]</code> is the pairwise predictive density for margins 1 and 2 conditioned by $K = 1$ , <code>dens[[1]][[2]] = dens[["1-2"]][[2]]</code> is the pairwise predictive density for margins 1 and 2 conditioned by $K = 2$ etc. Note that <code>densK</code> provides some additional information only when <code>Krandom = TRUE</code> or when <code>x</code> results from the <code>NMixMCMC</code> call to the reversible jump MCMC.

There is also a `plot` method implemented for the resulting object.

### Author(s)

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

### References

Komárek, A. (2009). A new R package for Bayesian estimation of multivariate normal mixtures allowing for selection of the number of components and interval-censored data. *Computational Statistics and Data Analysis*, **53**(12), 3932–3947.

**See Also**

[plot.NMixPredDensJoint2](#), [NMixMCMC](#), [GLMM\\_MCMC](#), [NMixPredDensMarg](#).

**Examples**

```
## See additional material available in
## YOUR_R_DIR/library/mixAK/doc/
## or YOUR_R_DIR/site-library/mixAK/doc/
## http://www.karlin.mff.cuni.cz/~komarek/software/mixAK/Galaxy.pdf
## http://www.karlin.mff.cuni.cz/~komarek/software/mixAK/Faithful.pdf
## http://www.karlin.mff.cuni.cz/~komarek/software/mixAK/Tandmob.pdf
##
```

---

NMixPredDensMarg	<i>Marginal (univariate) predictive density</i>
------------------	---

---

**Description**

This function serves as an inference tool for the MCMC output obtained using the function [NMixMCMC](#). It computes estimated posterior predictive densities for each margin.

**Usage**

```
NMixPredDensMarg(x, ...)

## Default S3 method:
NMixPredDensMarg(x, scale, K, w, mu, Li, Krandom=TRUE, ...)

## S3 method for class 'NMixMCMC'
NMixPredDensMarg(x, grid, lgrid=500, scaled=FALSE, ...)

## S3 method for class 'GLMM_MCMC'
NMixPredDensMarg(x, grid, lgrid=500, scaled=FALSE, ...)
```

**Arguments**

x	an object of class <code>NMixMCMC</code> for <code>NMixPredDensMarg.NMixMCMC</code> function. An object of class <code>GLMM_MCMC</code> for <code>NMixPredDensMarg.GLMM_MCMC</code> function. A list with the grid values (see below) for <code>NMixPredDensMarg.default</code> function.
scale	a two component list giving the shift and the scale.
K	either a number (when <code>Krandom=FALSE</code> ) or a numeric vector with the chain for the number of mixture components.
w	a numeric vector with the chain for the mixture weights.
mu	a numeric vector with the chain for the mixture means.



Li	a numeric vector with the chain for the mixture inverse variances (lower triangles only).
Krandom	a logical value which indicates whether the number of mixture components changes from one iteration to another.
grid	a numeric vector or a list with the grid values in which the predictive density should be evaluated. If $x_{dim}$ is 1 then grid may be a numeric vector. If $x_{dim}$ is higher than then grid must be a list with numeric vectors as components giving the grids for each margin. If grid is not specified, it is created automatically using the information from the posterior summary statistics stored in $x$ .
lgrid	a length of the grid used to create the grid if that is not specified.
scaled	if TRUE, the density of shifted and scaled data is summarized. The shift and scale vector are taken from the scale component of the object $x$ .
...	optional additional arguments.

### Value

An object of class `NMixPredDensMarg` which has the following components:

x	a list with the grid values for each margin. The components of the list are named $x_1, \dots$ or take names from grid argument.
freqK	frequency table for the values of $K$ (numbers of mixture components) in the MCMC chain.
propK	proportions derived from freqK.
MCMC.length	the length of the MCMC used to compute the predictive densities.
dens	a list with the computed predictive densities for each margin. The components of the list are named 1, ..., i.e., <code>dens[[1]] = dens[["1"]]</code> is the predictive density for margin 1 etc.
densK	a list with the computed predictive densities for each margin, conditioned further by $K$ . The components of the list are named 1, ... That is, <code>dens[[1]][[1]] = dens[["1"]][[1]]</code> is the predictive density for margin 1 conditioned by $K = 1$ , <code>dens[[1]][[2]] = dens[["1"]][[2]]</code> is the predictive density for margin 1 conditioned by $K = 2$ etc. Note that densK provides some additional information only when <code>Krandom = TRUE</code> or when $x$ results from the <code>NMixMCMC</code> call to the reversible jump MCMC.

There is also a `plot` method implemented for the resulting object.

### Author(s)

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

### References

Komárek, A. (2009). A new R package for Bayesian estimation of multivariate normal mixtures allowing for selection of the number of components and interval-censored data. *Computational Statistics and Data Analysis*, **53**(12), 3932–3947.

**See Also**

[plot.NMixPredDensMarg](#), [NMixMCMC](#), [GLMM\\_MCMC](#), [NMixPredDensJoint2](#).

**Examples**

```
## See additional material available in
## YOUR_R_DIR/library/mixAK/doc/
## or YOUR_R_DIR/site-library/mixAK/doc/
## http://www.karlin.mff.cuni.cz/~komarek/software/mixAK/Galaxy.pdf
## http://www.karlin.mff.cuni.cz/~komarek/software/mixAK/Faithful.pdf
## http://www.karlin.mff.cuni.cz/~komarek/software/mixAK/Tandmob.pdf
##
```

---

NMixPseudoGOF

*Pseudo goodness-of-fit test for a normal mixture model*

---

**Description**

It takes a (fitted) normal mixture, creates hyperrectangles according to a specified grid, computes probability masses in each hyperrectangle derived from the (fitted) normal mixture. From computed probability masses expected frequencies (using the sample size of supplied data) are computed and compared to frequencies observed in supplied data. From expected and observed frequencies, a Pearson chi-squared like statistic is computed and returned together with residuals derived from that statistic.

Also pseudo degrees of freedom are returned which are equal to a number of hyperrectangles minus number of free parameters of the normal mixture. For a  $K$ -component mixture of dimension  $p$ , the number of free parameters is computed as

$$q = K - 1 + K \cdot p + K \cdot p(p + 1)/2$$

Note that computation of  $q$  does not take into account the positive (semi-)definiteness restriction on covariance matrices.

**WARNING:** There is no statistical theory developed that would guarantee that computed chi-squared like statistics follows a chi-squared distribution with computed pseudo degrees of freedom under the null hypothesis that the distribution that generated the data is a normal mixture. This function serves purely for descriptive purposes!

**Usage**

```
NMixPseudoGOF(x, ...)
```

## Default S3 method:

```
NMixPseudoGOF(x, scale, w, mu, Sigma, breaks, nbreaks=10, digits=3, ...)
```

## S3 method for class 'NMixMCMC'

```
NMixPseudoGOF(x, y, breaks, nbreaks=10, digits=3, ...)
```

**Arguments**

<code>x</code>	data object (see argument <code>y</code> below) for <code>NMixPseudoGOF.default</code> function. An object of class <code>NMixMCMC</code> for <code>NMixPseudoGOF.NMixMCMC</code> function.
<code>y</code>	a numeric vector, matrix or data frame with the data. It is a numeric vector if $p$ is one. It is a matrix or data frame with $p$ columns if $p > 1$ .
<code>scale</code>	a two component list giving the <code>shift</code> and the <code>scale</code> . If not given, <code>shift</code> is equal to zero and <code>scale</code> is equal to one.
<code>w</code>	a numeric vector with mixture weights. The length of this vector determines the number of mixture components.
<code>mu</code>	a matrix with mixture means in rows. That is, <code>mu</code> has $K$ rows and $p$ columns, where $K$ denotes the number of mixture components and $p$ is dimension of the mixture distribution.
<code>Sigma</code>	a list with mixture covariance matrices.
<code>breaks</code>	a numeric vector or a list with the breaks defining the hyperrectangles. It is a numeric vector if $p$ is equal to one. It is a list of length $p$ of numeric vectors. Each component of the list determines the breaks for each margin.
<code>nbreaks</code>	a number or a numeric vector with the number of breaks for each margin. It is only used if the argument <code>breaks</code> is not given to determine sensible break values.
<code>digits</code>	a number or a numeric vector with the number of digits to which the breaks should be rounded in the case they are created by the function. If it is a vector then different rounding may be used for each margin.
<code>...</code>	optional additional arguments.

**Value**

ADD DESCRIPTION

**Author(s)**

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

**See Also**

[NMixMCMC](#).

## Description

This function takes an object generated by the `NMixMCMC` or `GLMM_MCMC` function and internally re-labels the mixture components using selected re-labeling algorithm. It also computes posterior summary statistics for mixture means, weights, variances which correspond to newly labeled MCMC sample. Further, posterior component probabilities (`poster.comp.prob_u` and `poster.comp.prob_b` components of the object object) are updated according to the newly labeled MCMC sample.

This function only works for models with a fixed number of mixture components.

## Usage

```
NMixRelabel(object, type=c("mean", "weight", "stephens"), par, ...)

## Default S3 method:
NMixRelabel(object, type = c("mean", "weight", "stephens"), par, ...)

## S3 method for class 'NMixMCMC'
NMixRelabel(object, type = c("mean", "weight", "stephens"), par,
  prob=c(0.025, 0.5, 0.975), keep.comp.prob = FALSE, info, ...)

## S3 method for class 'NMixMCMClist'
NMixRelabel(object, type = c("mean", "weight", "stephens"), par,
  prob=c(0.025, 0.5, 0.975), keep.comp.prob = FALSE, info,
  silent = FALSE, parallel = FALSE, ...)

## S3 method for class 'GLMM_MCMC'
NMixRelabel(object, type = c("mean", "weight", "stephens"), par,
  prob = c(0.025, 0.5, 0.975), keep.comp.prob = FALSE, info,
  silent = FALSE, ...)

## S3 method for class 'GLMM_MCMClist'
NMixRelabel(object, type = c("mean", "weight", "stephens"), par,
  prob = c(0.025, 0.5, 0.975), keep.comp.prob = FALSE, jointly = FALSE,
  info, silent = FALSE, parallel = FALSE, ...)
```

## Arguments

<code>object</code>	an object of appropriate class.
<code>type</code>	character string which specifies the type of the re-labeling algorithm.
<code>par</code>	additional parameters for particular re-labeling algorithms.
	<b>mean</b> <code>par</code> specifies margin which is used to order the components. It is set to 1 if not given.
	<b>weight</b> <code>par</code> is empty.
	<b>stephens</b> <code>par</code> is a list with components <code>type.init</code> , <code>par</code> , <code>maxiter</code> . Component <code>type.init</code> is a character string being equal to either of “identity”, “mean”, “weight”. It determines the way which is used to obtain initial re-labeling.

	Component <code>par</code> determines the margin in the case that <code>type.init</code> is equal to “mean”.
	Component <code>max.iter</code> determines maximum number of iterations of the re-labeling algorithm.
<code>prob</code>	probabilities for which the posterior quantiles of component allocation probabilities are computed.
<code>keep.comp.prob</code>	logical. If TRUE, posterior sample of component allocation probabilities (for each subject) is kept in the resulting object.
<code>jointly</code>	a logical value. If it is TRUE then both chains are processed together. In the output, all posterior summary statistics are then also related to both chains as if it is one long chain. If it is FALSE then both chains are processed independently.
<code>info</code>	number which specifies frequency used to re-display the iteration counter during the computation.
<code>silent</code>	a logical value indicating whether the information on the MCMC progress is to be suppressed.
<code>parallel</code>	a logical value indicating whether parallel computation (based on a package <code>parallel</code> ) should be used (if possible) for re-labelling of the two chains.
<code>...</code>	optional additional arguments.

### Value

An object being equal to the value of the `object` argument in which the following components are updated according to new labeling of the mixture components.

### Value for NMixMCMC object

When the argument `object` is of class `NMIXMCMC`, the resulting object is equal to `object` with the following components being modified:

**relabel** see [NMIXMCMC](#)  
**order** see [NMIXMCMC](#)  
**rank** see [NMIXMCMC](#)  
**poster.mean.w** see [NMIXMCMC](#)  
**poster.mean.mu** see [NMIXMCMC](#)  
**poster.mean.Q** see [NMIXMCMC](#)  
**poster.mean.Sigma** see [NMIXMCMC](#)  
**poster.mean.Li** see [NMIXMCMC](#)  
**poster.comp.prob\_u** see [NMIXMCMC](#)  
**poster.comp.prob\_b** see [NMIXMCMC](#)

Additionally, new components are added, namely

**quant.comp.prob\_b** a list with the posterior quantiles of component probabilities. One list component for each quantile specified by `prob` argument.

**comp.prob\_b** posterior sample of individual component probabilities (also given random effects). It is an  $M \times n \cdot K$  matrix where  $M$  is the length of the posterior sample,  $n$  is the number of subjects, and  $K$  is the number of mixture components. Component labels correspond to the re-labelled sample. It is included in the resulting object only if `keep.comp.prob` argument is TRUE.

### Value for GLMM\_MCMC object

When the argument object is of class `GLMM_MCMC`, the resulting object is equal to object with the following components being modified:

**relabel\_b** see [GLMM\\_MCMC](#)

**order\_b** see [GLMM\\_MCMC](#)

**rank\_b** see [GLMM\\_MCMC](#)

**poster.mean.w\_b** see [GLMM\\_MCMC](#)

**poster.mean.mu\_b** see [GLMM\\_MCMC](#)

**poster.mean.Q\_b** see [GLMM\\_MCMC](#)

**poster.mean.Sigma\_b** see [GLMM\\_MCMC](#)

**poster.mean.Li\_b** see [GLMM\\_MCMC](#)

**poster.comp.prob\_u** see [GLMM\\_MCMC](#)

**poster.comp.prob\_b** see [GLMM\\_MCMC](#)

Additionally, new components are added, namely

**quant.comp.prob\_b** a list with the posterior quantiles of component probabilities. One list component for each quantile specified by `prob` argument.

**comp.prob\_b** posterior sample of individual component probabilities (also given random effects). It is an  $M \times I \cdot K$  matrix where  $M$  is the length of the posterior sample,  $I$  is the number of subjects, and  $K$  is the number of mixture components. Component labels correspond to the re-labelled sample. It is included in the resulting object only if `keep.comp.prob` argument is TRUE.

**poster.comp.prob** a matrix with the posterior means of component probabilities which are calculated with random effects integrated out.

**quant.comp.prob** a list with the posterior quantiles of component probabilities. One list component for each quantile specified by `prob` argument.

**comp.prob** posterior sample of individual component probabilities (with random effects integrated out). It is an  $M \times I \cdot K$  matrix where  $M$  is the length of the posterior sample,  $I$  is the number of subjects, and  $K$  is the number of mixture components. Component labels correspond to the re-labelled sample. It is included in the resulting object only if `keep.comp.prob` argument is TRUE.

**Remark.** These are the component probabilities which should normally be used for clustering purposes.

### Author(s)

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

## References

- Celeux, G. (1998). Bayesian inference for mixtures: The label-switching problem. In: *COMPSTAT 98* (eds. R. Payne and P. Green), pp. 227-232. Heidelberg: Physica-Verlag.
- Jasra, A., Holmes, C. C., and Stephens, D. A. (2005). Markov chain Monte Carlo methods and the label switching problem in Bayesian mixture modeling. *Statistical Science*, **20**, 50-67.
- Stephens, M. (1997). *Bayesian methods for mixtures of normal distributions*. DPhil Thesis. Oxford: University of Oxford. (Available from: <http://stephenslab.uchicago.edu/publications.html> (accessed on 05/02/2014)).
- Stephens, M. (2000). Dealing with label switching in mixture models. *Journal of the Royal Statistical Society, Series B*, **62**, 795-809.

## See Also

[NMixMCMC](#), [GLMM\\_MCMC](#).

## Examples

```
## See also additional material available in
## YOUR_R_DIR/library/mixAK/doc/
## or YOUR_R_DIR/site-library/mixAK/doc/
## - file PBCseq.R and
##   http://www.karlin.mff.cuni.cz/~komarek/software/mixAK/PBCseq.pdf
##
## =====
```

---

NMixSummComp

*Summary for the mixture components*

---

## Description

This function returns basic posterior summary for (re-labeled) mixture components in a model with fixed number of components fitted with [NMixMCMC](#) or [GLMM\\_MCMC](#) function. The summary also takes into account possible scaling and shifting of the data (see argument `scale` in [NMixMCMC](#) function or argument `scale.b` in [GLMM\\_MCMC](#)).

Note that even though the mixture components are re-labeled before the summary is computed to achieve some identifiability, posterior summaries of individual mixture means and variances are not always the quantity we would like to see. For density estimation, posterior predictive density ([NMixPredDensMarg](#), [NMixPredDensJoint2](#)) is usually the right stuff one should be interested in.

## Usage

```
NMixSummComp(x)

## Default S3 method:
NMixSummComp(x)
```

```
## S3 method for class 'NMixMCMC'  
NMixSummComp(x)
```

```
## S3 method for class 'GLMM_MCMC'  
NMixSummComp(x)
```

### Arguments

`x` an object of class `NMixMCMC` or `GLMM_MCMC`

### Value

Invisible `x`. The rest is printed on output device.

### Author(s)

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

### See Also

[NMixMCMC](#), [GLMM\\_MCMC](#).

---

PBC910

*Subset of Mayo Clinic Primary Biliary Cirrhosis data*

---

### Description

This is a subset of [PBCseq](#) data which contains only data from 260 patients known to be alive and without liver transplantation at 910 days of follow-up. Furthermore, only a selection of longitudinal measurements is included and only those measurements that were obtained by 910 days. The PBC910 dataset was used in papers Komárek and Komárková (2013, 2014).

### Usage

```
data(PBCseq)
```

### Format

a data frame with 918 rows and the following variables

**id** identification number of a patient

**day** number of days between enrollment and this visit date (all measurements below refer to this date)

**month** number of months between enrollment and this visit date

**fu.days** total number of follow up days

**delta.ltx.death** 0/1 censoring indicator for event = death or liver transplantation related to `fu.days`

**lbili** natural logarithm of above



**platelet** platelet count  
**spiders** 0/1 presence of blood vessel malformations in the skin  
**jspiders** jittered version of a variable spiders

### Source

URL: <http://lib.stat.cmu.edu/datasets/>

### References

Komárek, A. and Komárková, L. (2013). Clustering for multivariate continuous and discrete longitudinal data. *The Annals of Applied Statistics*, **7**(1), 177–200.

Komárek, A. and Komárková, L. (2014). Capabilities of R package mixAK for clustering based on multivariate continuous and discrete longitudinal data. *Journal of Statistical Software*, **59**(12), 1–38. <http://www.jstatsoft.org/v59/i12/>.

### See Also

[PBC910](#), [pbc](#), [pbcseq](#)

### Examples

```
data(PBC910)
summary(PBC910)
```

---

PBCseq

*Mayo Clinic Primary Biliary Cirrhosis, sequential data*

---

### Description

This data is a continuation of the PBC data set ([pbc](#)), and contains the follow-up laboratory data for each study patient. An analysis based on the data can be found in Murtagh et al. (1994).

The primary PBC data set contains only baseline measurements of the laboratory parameters. This data set contains multiple laboratory results, but only on the 312 randomized patients. Some baseline data values in this file differ from the original PBC file, for instance, the data errors in prothrombin time and age which were discovered after the original analysis (see Fleming and Harrington, 1991, figure 4.6.7).

### Usage

```
data(PBCseq)
```

**Format**

a data frame with 1 945 rows and the following variables

**id** identification number of a patient

**sex** 0/1 for male and female

**fsex** factor of above

**drug** 0/1 for placebo and D-penicillamine

**fdrug** factor of above

**age** age at entry in years

**fu.days** total number of follow up days

**alive** number of days when the patient is known to be alive and without liver transplantation

**status** status at endpoint, 0/1/2 for censored, liver transplant, dead

**fstatus** factor of above

**delta.death** 0/1 censoring indicator for event = death (i.e., liver transplantation means censoring)

**delta.ltx.death** 0/1 censoring indicator for event = death or liver transplantation

**day** number of days between enrollment and this visit date (all measurements below refer to this date)

**month** number of months between enrollment and this visit date

**ascites** 0/1 presence of ascites

**fascites** factor of above

**hepatom** 0/1 presence of hepatomegaly or enlarged liver

**fhepatom** factor of above

**spiders** 0/1 presence of blood vessel malformations in the skin

**fspiders** factor of above

**edema** presence and status of edema, 0 for no edema, 0.5 for untreated or successfully treated edema, 1 for edema despite diuretic therapy

**fedema** factor of above

**stage** histologic stage of disease (needs biopsy)

**fstage** factor of above

**bili** serum bilirubin (mg/dl)

**lbili** natural logarithm of above

**albumin** serum albumin (mg/dl)

**lalbumin** natural logarithm of above

**alk.phos** alkaline phosphatase (U/liter)

**lalk.phos** natural logarithm of above

**chol** serum cholesterol (mg/dl)

**lchol** natural logarithm of above

**sgot** serum glutamic-oxaloacetic transaminase (the enzyme name has subsequently changed to "ALT" in the medical literature) (U/ml)

**lsgot** natural logarithm of above  
**platelet** platelet count  
**lplatelet** natural logarithm of above  
**prottime** standardised blood clotting time  
**lprottime** natural logarithm of above

### Source

URL: <http://lib.stat.cmu.edu/datasets/>

### References

- Dickson, E. R., Grambsch, P. M., Fleming, T. R., Fisher, L. D., and Langworthy, A. (1989). Prognosis in primary biliary-cirrhosis – Model for decision-making. *Hepatology*, **10**, 1–7.
- Fleming, T. R. and Harrington, D. P. (1991). *Counting Processes and Survival Analysis*. New York: John Wiley and Sons.
- Markus, B. H., Dickson, E. R., Grambsch, P. M., Fleming, T. R., Mazzaferro, V., Klintmalm, G. B. G., Wiesner, R. H., Vanthiel, D. H., and Starzl, T. E. (1989). Efficacy of liver-transplantation in patients with primary biliary-cirrhosis. *New England Journal of Medicine*, **320**, 1709–1713.
- Murtaugh, P. A., Dickson, E. R., Van Dam, G. M., Malinchoc, M., Grambsch, P. M., Langworthy, A. L., and Gips, C. H. (1994). Primary biliary cirrhosis: Prediction of short-term survival based on repeated patient visits. *Hepatology*, **20**, 126-134.
- Therneau, T. M. and Grambsch, P. M. (2000). *Modeling Survival Data: Extending the Cox Model*. New York: Springer-Verlag.

### See Also

[pbc](#), [pbcseq](#)

### Examples

```
data(PBCseq)
summary(PBCseq)
```

---

```
plot.NMixPlugCondDensJoint2
```

*Plot computed pairwise bivariate conditional densities (plug-in estimate)*

---

### Description

This is a basic plotting tool to visualize computed plug-in estimates of pairwise bivariate conditional densities using the [image](#) or [contour](#) plot. See also [NMixPlugCondDensJoint2](#).

**Usage**

```
## S3 method for class 'NMixPlugCondDensJoint2'
plot(x, ixcond, imargin,
     contour=FALSE,
     add.contour=TRUE, col.add.contour="brown",
     auto.layout=TRUE,
     col, lwd=1, main, xylab, ...)
```

**Arguments**

<code>x</code>	an object of class <code>NMixPlugCondDensJoint2</code> .
<code>ixcond</code>	if given then conditional densities of all pairs of margins given <code>x[[ixcond]][ixcond]</code> are plotted where <code>ixcond</code> is taken from <code>x</code> .
<code>imargin</code>	vector of length 2. if given then conditional densities of the ( <code>imargin[1]</code> , <code>imargin[2]</code> ) pair of margins given all values of <code>x[[ixcond]]</code> are plotted.
<code>contour</code>	logical. If <code>TRUE</code> then contours are drawn, otherwise image plot is created.
<code>add.contour</code>	logical. If <code>TRUE</code> and <code>contour</code> is <code>FALSE</code> (i.e., image plot is drawn) then contours are added to the image plots.
<code>col.add.contour</code>	color of contours which are added to the image plot.
<code>auto.layout</code>	if <code>TRUE</code> then the function determines itself how to divide the plotting region to draw densities for all margins.
<code>col</code>	color used to draw the contours or images.
<code>lwd</code>	line width.
<code>main</code>	main title of the plot.
<code>xylab</code>	optional character vector of the length equal to the number of margins with labels used for x and y axes on the plots.
<code>...</code>	additional arguments passed to the plot function.

**Value**

`invisible(x)`

**Author(s)**

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

**See Also**

[NMixPlugCondDensJoint2](#), [NMixMCMC](#).

---

plot.NMixPlugCondDensMarg

*Plot computed univariate conditional densities (plug-in estimate)*


---

### Description

This is a basic plotting tool to visualize computed plug-in estimates of univariate conditional densities, see [NMixPlugCondDensMarg](#).

### Usage

```
## S3 method for class 'NMixPlugCondDensMarg'
plot(x, ixcond, imargin, over=FALSE,
     auto.layout=TRUE, type="l", lwd=1, lty, col, main, xlab, ylab, ylim,
     annot=TRUE, ...)
```

### Arguments

x	an object of class NMixPlugCondDensMarg.
ixcond	if given then conditional densities of all margins given $x[[i\text{cond}]]$ are plotted where $i\text{cond}$ is taken from $x$ .
imargin	if given then conditional densities of the $i\text{margin}$ -th margin given all values of $x[[i\text{cond}]]$ are plotted - either separately or all in one plot.
over	logical. If TRUE and $i\text{margin}$ is given then all conditional densities are drawn in one plot.
auto.layout	if TRUE then the function determines itself how to divide the plotting region to draw the computed densities.
type	type of the plot.
lwd	line width.
col	color used to draw the lines. It can be a vector in which case different lines are drawn in different colors.
lty	type of the line. It can be a vector in which case different lines are drawn in different types.
main	main title of the plot. Either character which is replicated or a vector of characters.
xlab	label for the x-axis. Either character which is replicated or a vector of characters.
ylab	label for the y-axis. Either character which is replicated or a vector of characters.
ylim	limits for the y-axis.
annot	if TRUE and $i\text{margin}$ is given and $over$ is TRUE then a legend is added to the plot.
...	additional arguments passed to the plot function.

**Value**

invisible(x)

**Author(s)**

Arnošt Komárek &lt;arnost.komarek[AT]mff.cuni.cz&gt;

**See Also**[NMixPlugCondDensMarg](#), [NMixMCMC](#).

---

`plot.NMixPlugDensJoint2`*Plot computed marginal pairwise bivariate densities (plug-in estimate)*

---

**Description**

This is a basic plotting tool to visualize computed marginal pairwise bivariate densities (plug-in version) using the [contour](#) plot. See also [NMixPlugDensJoint2](#).

**Usage**

```
## S3 method for class 'NMixPlugDensJoint2'
plot(x, contour=FALSE,
     add.contour=TRUE, col.add.contour="brown",
     auto.layout=TRUE,
     col, lwd=1, main, xylab, ...)
```

**Arguments**

<code>x</code>	an object of class <code>NMixPlugDensJoint2</code> .
<code>contour</code>	logical. If TRUE then contours are drawn, otherwise image plot is created.
<code>add.contour</code>	logical. If TRUE and <code>contour</code> is FALSE (i.e., image plot is drawn) then contours are added to the image plots.
<code>col.add.contour</code>	color of contours which are added to the image plot.
<code>auto.layout</code>	if TRUE then the function determines itself how to divide the plotting region to draw densities for all margins.
<code>col</code>	color used to draw the contours or images.
<code>lwd</code>	line width.
<code>main</code>	main title of the plot.
<code>xylab</code>	optional character vector of the length equal to the number of margins with labels used for x and y axes on the plots.
<code>...</code>	additional arguments passed to the <code>plot</code> function.

**Value**

invisible(x)

**Author(s)**

Arnošt Komárek &lt;arnost.komarek[AT]mff.cuni.cz&gt;

**See Also**[NMixPlugDensJoint2](#), [NMixMCMC](#).

---

plot.NMixPlugDensMarg *Plot computed marginal predictive densities*


---

**Description**

This is a basic plotting tool to visualize computed marginal plug-in estimates of densities, see [NMixPlugDensMarg](#).

**Usage**

```
## S3 method for class 'NMixPlugDensMarg'
plot(x, auto.layout=TRUE,
     type="l", col="darkblue", lty=1, lwd=1, main, xlab, ylab, ...)
```

**Arguments**

x	an object of class <code>NMixPlugDensMarg</code> .
auto.layout	if TRUE then the function determines itself how to divide the plotting region to draw densities for all margins.
type	type of the plot.
col	color used to draw the lines.
lty	type of the line.
lwd	line width.
main	main title of the plot. Either character which is replicated or a vector of characters of the length equal to the number of margins.
xlab	label for the x-axis. Either character which is replicated or a vector of characters of the length equal to the number of margins.
ylab	label for the y-axis. Either character which is replicated or a vector of characters of the length equal to the number of margins.
...	additional arguments passed to the <code>plot</code> function.

**Value**

invisible(x)

**Author(s)**

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

**See Also**

[NMixPlugDensMarg](#), [NMixMCMC](#).

---

plot.NMixPredCDFMarg *Plot computed marginal predictive cumulative distribution functions*

---

**Description**

This is a basic plotting tool to visualize computed marginal cumulative distribution functions, see [NMixPredCDFMarg](#).

**Usage**

```
## S3 method for class 'NMixPredCDFMarg'
plot(x, K=0, auto.layout=TRUE,
     type="l", col="darkblue", lty=1, lwd=1, main, xlab, ylab, ...)
```

**Arguments**

x	an object of class NMixPredCDFMarg.
K	if equal to 0 then the overall predictive CDF's are plotted taken from the dens part of the object x. If higher than 0 then the predictive CDF conditioned by the value of K is plotted (taken from the densK part of the object x).
auto.layout	if TRUE then the function determines itself how to divide the plotting region to draw densities for all margins.
type	type of the plot.
col	color used to draw the lines.
lty	type of the line.
lwd	line width.
main	main title of the plot. Either character which is replicated or a vector of characters of the length equal to the number of margins.
xlab	label for the x-axis. Either character which is replicated or a vector of characters of the length equal to the number of margins.
ylab	label for the y-axis. Either character which is replicated or a vector of characters of the length equal to the number of margins.
...	additional arguments passed to the plot function.



**Value**

invisible(x)

**Author(s)**

Arnošt Komárek &lt;arnost.komarek[AT]mff.cuni.cz&gt;

**References**

Komárek, A. (2009). A new R package for Bayesian estimation of multivariate normal mixtures allowing for selection of the number of components and interval-censored data. *Computational Statistics and Data Analysis*, **53**(12), 3932–3947.

**See Also**

[NMixPredCDFMarg](#), [NMixMCMC](#).

plot.NMixPredCondCDFMarg

*Plot computed univariate conditional predictive cumulative distribution functions*

**Description**

This is a basic plotting tool to visualize computed posterior predictive estimates of univariate conditional cdf's, see [NMixPredCondCDFMarg](#).

**Usage**

```
## S3 method for class 'NMixPredCondCDFMarg'
plot(x, ixcond, imargin, prob, over=FALSE,
     auto.layout=TRUE, type="l", lwd=1, lty, col, qlwd=1, qlty, qcol,
     main, xlab, ylab, ylim,
     annot=TRUE, ...)
```

**Arguments**

x	an object of class NMixPredCondCDFMarg.
ixcond	if given then conditional cdf's of all margins given x[[ixcond]][ixcond] are plotted where ixcond is taken from x.
imargin	if given then conditional cdf's of the imargin-th margin given all values of x[[ixcond]] are plotted - either separately or all in one plot.
prob	probabilities of pointwise posterior quantiles which should be added to the plot. Computed values of requested posterior quantiles must be present in the object x (see argument prob of <a href="#">NMixPredCondCDFMarg</a> ).

over	logical. If TRUE and imargin is given then all conditional cdf's are drawn in one plot.
auto.layout	if TRUE then the function determines itself how to divide the plotting region to draw the computed cdf's.
type	type of the plot.
lwd	line width.
lty	type of the line. It can be a vector in which case different lines are drawn in different types.
col	color used to draw the lines. It can be a vector in which case different lines are drawn in different colors.
qlwd	line width for pointwise posterior quantiles.
qlty	type of the line for pointwise posterior quantiles.
qcol	color used to draw pointwise posterior quantiles.
main	main title of the plot. Either character which is replicated or a vector of characters.
xlab	label for the x-axis. Either character which is replicated or a vector of characters.
ylab	label for the y-axis. Either character which is replicated or a vector of characters.
ylim	limits for the y-axis.
annot	if TRUE and imargin is given and over is TRUE then a legend is added to the plot.
...	additional arguments passed to the plot function.

**Value**

invisible(x)

**Author(s)**

Arnošt Komárek &lt;arnost.komarek[AT]mff.cuni.cz&gt;

**See Also**[NMixPredCondCDFMarg](#), [NMixMCMC](#).

---

plot.NMixPredCondDensJoint2
*Plot computed predictive pairwise bivariate conditional densities*


---

**Description**

This is a basic plotting tool to visualize computed predictive pairwise bivariate conditional densities using the [image](#) or [contour](#) plot. See also [NMixPredCondDensJoint2](#).

**Usage**

```
## S3 method for class 'NMixPredCondDensJoint2'
plot(x, ixcond, imargin,
     contour=FALSE,
     add.contour=TRUE, col.add.contour="brown",
     auto.layout=TRUE,
     col, lwd=1, main, xylab, ...)
```

**Arguments**

x	an object of class NMixPredCondDensJoint2.
ixcond	if given then conditional densities of all pairs of margins given $x[[ixcond]][ixcond]$ are plotted where ixcond is taken from x.
imargin	vector of length 2. if given then conditional densities of the (imargin[1], imargin[2]) pair of margins given all values of $x[[ixcond]]$ are plotted.
contour	logical. If TRUE then contours are drawn, otherwise image plot is created.
add.contour	logical. If TRUE and contour is FALSE (i.e., image plot is drawn) then contours are added to the image plots.
col.add.contour	color of contours which are added to the image plot.
auto.layout	if TRUE then the function determines itself how to divide the plotting region to draw densities for all margins.
col	color used to draw the contours or images.
lwd	line width.
main	main title of the plot.
xylab	optional character vector of the length equal to the number of margins with labels used for x and y axes on the plots.
...	additional arguments passed to the plot function.

**Value**

invisible(x)

**Author(s)**

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

**See Also**

[NMixPredCondDensJoint2](#), [NMixMCMC](#).

---

```
plot.NMixPredCondDensMarg
```

*Plot computed univariate conditional predictive densities*

---

## Description

This is a basic plotting tool to visualize computed posterior predictive estimates of univariate conditional densities, see [NMixPredCondDensMarg](#).

## Usage

```
## S3 method for class 'NMixPredCondDensMarg'
plot(x, ixcond, imargin, prob, over=FALSE,
     auto.layout=TRUE, type="l", lwd=1, lty, col, qlwd=1, qlty, qcol,
     main, xlab, ylab, ylim,
     annot=TRUE, ...)
```

## Arguments

x	an object of class <code>NMixPredCondDensMarg</code> .
ixcond	if given then conditional densities of all margins given <code>x[[ixcond]]</code> are plotted where <code>ixcond</code> is taken from <code>x</code> .
imargin	if given then conditional densities of the <code>imargin</code> -th margin given all values of <code>x[[ixcond]]</code> are plotted - either separately or all in one plot.
prob	probabilities of pointwise posterior quantiles which should be added to the plot. Computed values of requested posterior quantiles must be present in the object <code>x</code> (see argument <code>prob</code> of <a href="#">NMixPredCondDensMarg</a> ).
over	logical. If <code>TRUE</code> and <code>imargin</code> is given then all conditional densities are drawn in one plot.
auto.layout	if <code>TRUE</code> then the function determines itself how to divide the plotting region to draw the computed densities.
type	type of the plot.
lwd	line width.
lty	type of the line. It can be a vector in which case different lines are drawn in different types.
col	color used to draw the lines. It can be a vector in which case different lines are drawn in different colors.
qlwd	line width for pointwise posterior quantiles.
qlty	type of the line for pointwise posterior quantiles.
qcol	color used to draw pointwise posterior quantiles.
main	main title of the plot. Either character which is replicated or a vector of characters.

xlab	label for the x-axis. Either character which is replicated or a vector of characters.
ylab	label for the y-axis. Either character which is replicated or a vector of characters.
ylim	limits for the y-axis.
annot	if TRUE and imargin is given and over is TRUE then a legend is added to the plot.
...	additional arguments passed to the plot function.

**Value**

invisible(x)

**Author(s)**

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

**See Also**

[NMixPredCondDensMarg](#), [NMixMCMC](#).

---

plot.NMixPredDensJoint2

*Plot computed marginal pairwise bivariate predictive densities*

---

**Description**

This is a basic plotting tool to visualize computed marginal pairwise bivariate predictive densities using the [image](#) plot or [contour](#) plot. See also [NMixPredDensJoint2](#).

**Usage**

```
## S3 method for class 'NMixPredDensJoint2'
plot(x, K=0, contour=FALSE,
     add.contour=TRUE, col.add.contour="brown",
     auto.layout=TRUE,
     col, lwd=1, main, xylab, ...)
```

**Arguments**

x	an object of class NMixPredDensJoint2.
K	if equal to 0 then the overall predictive densities are plotted taken from the dens part of the object x. If higher than 0 then the predictive density conditioned by the value of K is plotted (taken from the densK part of the object x).
contour	logical. If TRUE then contours are drawn, otherwise image plot is created.
add.contour	logical. If TRUE and contour is FALSE (i.e., image plot is drawn) then contours are added to the image plots.

col.add.contour	color of contours which are added to the image plot.
auto.layout	if TRUE then the function determines itself how to divide the plotting region to draw densities for all margins.
col	color used to draw the contours or images.
lwd	line width.
main	main title of the plot.
xylab	optional character vector of the length equal to the number of margins with labels used for x and y axes on the plots.
...	additional arguments passed to the plot function.

**Value**

invisible(x)

**Author(s)**

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

**References**

Komárek, A. (2009). A new R package for Bayesian estimation of multivariate normal mixtures allowing for selection of the number of components and interval-censored data. *Computational Statistics and Data Analysis*, **53**(12), 3932–3947.

**See Also**

[NMixPredDensJoint2](#), [NMixMCMC](#).

**Examples**

```
## See additional material available in
## YOUR_R_DIR/library/mixAK/doc/
## or YOUR_R_DIR/site-library/mixAK/doc/
## - files Galaxy.R, Faithful.R, Tandmob.R and
## http://www.karlin.mff.cuni.cz/~komarek/software/mixAK/Galaxy.pdf
## http://www.karlin.mff.cuni.cz/~komarek/software/mixAK/Faithful.pdf
## http://www.karlin.mff.cuni.cz/~komarek/software/mixAK/Tandmob.pdf
```

---

plot.NMixPredDensMarg *Plot computed marginal predictive densities*

---

### Description

This is a basic plotting tool to visualize computed marginal predictive densities, see [NMixPredDensMarg](#).

### Usage

```
## S3 method for class 'NMixPredDensMarg'
plot(x, K=0, auto.layout=TRUE,
      type="l", col="darkblue", lty=1, lwd=1, main, xlab, ylab, ...)
```

### Arguments

x	an object of class NMixPredDensMarg.
K	if equal to 0 then the overall predictive densities are plotted taken from the dens part of the object x. If higher than 0 then the predictive density conditioned by the value of K is plotted (taken from the densK part of the object x).
auto.layout	if TRUE then the function determines itself how to divide the plotting region to draw densities for all margins.
type	type of the plot.
col	color used to draw the lines.
lty	type of the line.
lwd	line width.
main	main title of the plot. Either character which is replicated or a vector of characters of the length equal to the number of margins.
xlab	label for the x-axis. Either character which is replicated or a vector of characters of the length equal to the number of margins.
ylab	label for the y-axis. Either character which is replicated or a vector of characters of the length equal to the number of margins.
...	additional arguments passed to the plot function.

### Value

invisible(x)

### Author(s)

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

## References

Komárek, A. (2009). A new R package for Bayesian estimation of multivariate normal mixtures allowing for selection of the number of components and interval-censored data. *Computational Statistics and Data Analysis*, **53**(12), 3932–3947.

## See Also

[NMixPredDensMarg](#), [NMixMCMC](#).

## Examples

```
## See additional material available in
## YOUR_R_DIR/library/mixAK/doc/
## or YOUR_R_DIR/site-library/mixAK/doc/
## http://www.karlin.mff.cuni.cz/~komarek/software/mixAK/Galaxy.pdf
## http://www.karlin.mff.cuni.cz/~komarek/software/mixAK/Faithful.pdf
## http://www.karlin.mff.cuni.cz/~komarek/software/mixAK/Tandmob.pdf
##
```

---

plotProfiles

*Plot individual longitudinal profiles*

---

## Description

It creates a plot of individual longitudinal profiles. It is based on the output from `getProfiles` function.

## Usage

```
plotProfiles(ip, data, var, trans, tvar, gvar,
             auto.layout=TRUE, lines=TRUE, points=FALSE, add=FALSE,
             xlab="Time", ylab, xaxt="s", yaxt="s", xlim, ylim, main,
             lcol, col, bg, lty=1, lwd=1, pch=21, cex.points=1,
             highlight, lines.highlight=TRUE, points.highlight=TRUE,
             lcol.highlight="red3", col.highlight="red3", bg.highlight="orange",
             lty.highlight=1, lwd.highlight=2,
             pch.highlight=23, cex.highlight=1)
```

## Arguments

<code>ip</code>	output from <a href="#">getProfiles</a> function containing extracted individual longitudinal profiles of each subject.
<code>data</code>	<code>data.frame</code> used to produce <code>ip</code> . It is used to detect ranges for some variables.
<code>var</code>	character string identifying the response variable to plot.
<code>trans</code>	possible transformation of the response variable.



tvar	character string identifying the time variable.
gvar	character string identifying the group variable for which different colors are used.
auto.layout	logical. If TRUE, the layout of the plotting region is determined automatically.
lines	logical. If TRUE, lines are drawn in the plot connecting observations within individuals.
points	logical. If TRUE, points are added to the plot.
add	logical. If TRUE, the new plot overlays the old one.
lcol	color for lines.
col	color for points.
xlab, ylab, xaxt, yaxt, xlim, ylim, main, bg, lty, lwd, pch	arguments passed to standard plotting functions. col might also be a vector in which case different colors are used for profiles from different groups identified by the gvar variable.
cex.points	passed as a cex argument to <a href="#">points</a> function used when points = TRUE.
highlight	an optional numeric vector giving the indeces of ip for which the longitudinal profiles should be highlighted.
lines.highlight	logical. If TRUE, highlighting is done using lines.
points.highlight	logical. If TRUE, highlighting is done using points.
lcol.highlight, col.highlight, bg.highlight, lty.highlight, lwd.highlight, pch.highlight, cex.highlight	arguments col, bg, lty, lwd, pch, cex passed to <a href="#">lines</a> and/or <a href="#">points</a> functions which provide highlighting of selected profiles.

**Value**

Invisible ip.

**Author(s)**

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

**See Also**

[getProfiles](#).

**Examples**

```
data(PBCseq, package="mixAK")
ip <- getProfiles(t="day", y=c("age", "fdrug", "bili", "platelet", "spiders"),
                 id="id", data=PBCseq)
```

```
XLIM <- c(0, 910)
lcol2 <- c("darkgreen", "red")
```

```

oldPar <- par(mfrow=c(1, 3), bty="n")
plotProfiles(ip=ip, data=PBCseq, xlim=XLIM, var="bili", trans=log, tvar="day", gvar="fdrug",
             xlab="Time (days)", col=lcol2, auto.layout=FALSE, main="Log(bilirubin)",
             highlight=c(2, 4), col.highlight="darkblue")
plotProfiles(ip=ip, data=PBCseq, xlim=XLIM, var="platelet", tvar="day", gvar="fdrug",
             xlab="Time (days)", col=lcol2, auto.layout=FALSE, main="Platelet count",
             highlight=c(2, 4), col.highlight="darkblue")
plotProfiles(ip=ip, data=PBCseq, xlim=XLIM, var="spiders", tvar="day", gvar="fdrug",
             xlab="Time (days)", col=lcol2, auto.layout=FALSE,
             lines=FALSE, points=TRUE,
             highlight=c(2, 4), col.highlight="darkblue", bg.highlight="skyblue")
par(oldPar)

```

---

rRotationMatrix	<i>Random rotation matrix</i>
-----------------	-------------------------------

---

### Description

Generate a random rotation matrix, i.e., a matrix  $P = (p_{i,j})_{i=1,\dots,p,j=1,\dots,p}$ , which satisfies

- a)  $PP' = I$ ,
- b)  $P'P = I$ ,
- c)  $\det(P) = 1$ .

### Usage

```
rRotationMatrix(n, dim)
```

### Arguments

n	number of matrices to generate.
dim	dimension of a generated matrix/matrices.

### Details

For  $\text{dim} = 2$ ,  $p_{2,1}(\sin(\theta))$  is generated from  $\text{Unif}(0, 1)$  and the rest computed as follows:  $p_{1,1} = p_{2,2} = \sqrt{1 - p_{2,1}^2}(\cos(\theta))$  and  $p_{1,2} = -p_{2,1}(-\sin(\theta))$ .

For  $\text{dim} > 2$ , the matrix  $P$  is generated in the following steps:

- 1) Generate a  $p \times p$  matrix  $A$  with independent  $\text{Unif}(0, 1)$  elements and check whether  $A$  is of full rank  $p$ .
- 2) Computes a QR decomposition of  $A$ , i.e.,  $A = QR$  where  $Q$  satisfies  $QQ' = I$ ,  $Q'Q = I$ ,  $\det(Q) = (-1)^{p+1}$ , and columns of  $Q$  spans the linear space generated by the columns of  $A$ .
- 3) For odd  $\text{dim}$ , return matrix  $Q$ . For even  $\text{dim}$ , return corrected matrix  $Q$  to satisfy the determinant condition.

**Value**

For  $n=1$ , a matrix is returned.

For  $n>1$ , a list of matrices is returned.

**Author(s)**

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

**References**

Golub, G. H. and Van Loan, C. F. (1996, Sec. 5.1). *Matrix Computations. Third Edition*. Baltimore: The Johns Hopkins University Press.

**Examples**

```
P <- rRotationMatrix(n=1, dim=5)
print(P)
round(P %% t(P), 10)
round(t(P) %% P, 10)
det(P)

n <- 10
P <- rRotationMatrix(n=n, dim=5)
for (i in 1:3){
  cat(paste("*** i=", i, "\n", sep=""))
  print(P[[i]])
  print(round(P[[i]] %% t(P[[i]]), 10))
  print(round(t(P[[i]]) %% P[[i]], 10))
  print(det(P[[i]]))
}
```

---

rSamplePair

*Sample a pair (with replacement)*


---

**Description**

For given  $K$ , the function samples with replacement from a uniform distribution on a set of pairs  $(1, 2), (1, 3), \dots, (1, K), (2, 3), \dots, (2, K), \dots, (K - 1, K)$ .

**Usage**

```
rSamplePair(n, K)
```

**Arguments**

$n$                     number of pairs to sample.  
 $K$                     a numeric value which determines  $K$  (see above).

**Value**

A two-component numeric vector for  $n=2$  or a matrix with 2 columns with sampled pairs in rows for  $n>2$ .

**Author(s)**

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

**Examples**

```
rSamplePair(n=1, K=2)
rSamplePair(n=10, K=2)
```

```
rSamplePair(n=1, K=3)
rSamplePair(n=10, K=3)
```

```
rSamplePair(n=1, K=4)
rSamplePair(n=10, K=4)
```

---

SimData

*Simulated dataset*

---

**Description**

A simulated dataset used as an example dataset in Komárek and Komárková (2013+).

**Usage**

```
data(SimData)
```

**Format**

a data frame with 1 157 rows and the following variables

**id** identification number of a subject.

**tday** visit time in days.

**tmonth** visit time in months.

**yN** response variable generated according to a linear mixed model with normal errors. It intentionally contains 50 NA's.

**yP** response variable generated according to a Poisson generalized linear mixed model. It intentionally contains 50 NA's.

**yB** response variable generated according to a Bernoulli generalized linear mixed model. It intentionally contains 50 NA's.

**yBjit** a jittered version of yB.

## References

Komárek, A. and Komárková, L. (2013+). Capabilities of R package mixAK for clustering based on multivariate continuous and discrete longitudinal data. *Submitted*.

## Examples

```
data(SimData)
summary(SimData)
```

---

SP2Rect	<i>Conversion of a symmetric matrix stored in a packed format (lower triangle only) into a matrix</i>
---------	---

---

## Description

It creates a symmetric matrix from its lower triangle.

## Usage

```
SP2Rect(LT, dim)
```

## Arguments

LT	a numeric vector with the lower triangle (stored columnwise) of the matrix we want to reconstruct.
dim	number of rows and columns of a resulting matrix.

## Value

A matrix.

## Author(s)

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

## Examples

```
SP2Rect(3, dim=1)
SP2Rect(c(1, 0.5, 2), dim=2)
SP2Rect(c(1, 0.5, 0.25, 2, -0.5, 3), dim=3)
```

summaryDiff

*Posterior summary statistics for a difference of two quantities***Description**

It calculates (posterior) summary statistics for a difference of two quantities supplied as (MCMC) samples. Within `mixAK` package it is primarily used to calculate posterior summary for the difference of the deviances of two competing models.

**Usage**

```
summaryDiff(x, y, prob=c(0.025, 0.5, 0.975), cut=c(-2*log(9), 0), na.rm=TRUE)
```

**Arguments**

<code>x</code>	a numeric vector with the sample of the first quantity.
<code>y</code>	a numeric vector with the sample of the second quantity to be subtracted from <code>x</code> .
<code>prob</code>	a numeric vector of probabilities for quantiles to be calculated from the sample of differences.
<code>cut</code>	numeric value(s) which specify the cutoff(s) we are interested in estimating $P(x - y < \text{cut})$ from the sample. The default values are motivated by the arguments given in Section 4 of Aitkin, Liu and Chadwick (2009) and in Section 7.5 of Aitkin (2010).
<code>na.rm</code>	logical indicating on how to handle NA's.

**Value**

A list with the components

<code>summary</code>	a named vector with the (posterior) summary statistics based on the differences.
<code>Pcut</code>	estimated (posterior) probabilities that the difference lies below the cut values.

**Author(s)**

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

**References**

Aitkin, M. (2010). *Statistical Inference: An Integrated Bayesian/Likelihood Approach*. Boca Raton: CRC Press.

Aitkin, M., Liu, C. C., and Chadwick, T. (2009). Bayesian model comparison and model averaging for small-area estimation. *Annals of Applied Statistics*, **3**, 199-221.

## Examples

```
set.seed(16336886)
x <- runif(100, 0, 100)
y <- runif(100, 0, 100)
sdiff <- summaryDiff(x, y)
```

---

Tandmob

*Signal Tandmobiel data*

---

## Description

This is the dataset resulting from a longitudinal prospective dental study performed in Flanders (North of Belgium) in 1996 – 2001. The cohort of 4 468 randomly sampled children who attended the first year of the basic school at the beginning of the study was annually dental examined by one of 16 trained dentists. The original dataset consists thus of at most 6 dental observations for each child.

The dataset presented here contains mainly the information on the emergence and caries times summarized in the interval-censored observations. Some baseline covariates are also included here. This is a copy of [tandmob2](#) data in the package `bayesSurv`.

For more detail on the design of the study see Vanobbergen et al. (2000).

This data set was used in the analyses presented in Komárek et al. (2005), in Lesaffre, Komárek, and Declerck (2005) and in Komárek and Lesaffre (2007).

**IMPORTANT NOTICE:** It is possible to use these data for your research work under the condition that each manuscript is first approved by

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Belgium  
<emmanuel.lesaffre@med.kuleuven.be>

## Usage

```
data(Tandmob)
```

## Format

a data frame with 4 430 rows (38 sampled children did not come to any of the designed dental examinations) and the following variables

**IDNR** identification number of a child

**GENDER** character *boy* or *girl*

**GENDERNum** numeric, 0 = *boy*, 1 = *girl*

**DOB** character, date of birth in the format DDmmmYY

**PROVINCE** factor, code of the province with

- 0 = Antwerpen
- 1 = Vlaams Brabant
- 2 = Limburg
- 3 = Oost Vlaanderen
- 4 = West Vlaanderen

**EDUC** factor, code of the educational system with

- 0 = Free
- 1 = Community school
- 2 = Province/council school

**STARTBR** factor, code indicating the starting age of brushing the teeth (as reported by parents) with

- 1 = [0, 1] years
- 2 = (1, 2] years
- 3 = (2, 3] years
- 4 = (3, 4] years
- 5 = (4, 5] years
- 6 = later than at the age of 5

**FLUOR** binary covariate, 0 = no, 1 = yes. This is the covariate *fluorosis* used in the paper Komárek et al. (2005).

**BAD.xx** binary, indicator whether a deciduous tooth xx was removed because of orthodontical reasons or not.

xx takes values 53, 63, 73, 83 (deciduous lateral canines), 54, 64, 74, 84 (deciduous first molars), 55, 65, 75, 85 (deciduous second molars).

**EBEG.xx** lower limit of the emergence (in years of age) of the permanent tooth xx. NA if the emergence was left-censored.

xx takes values 11, 21, 31, 41 (permanent incisors), 12, 22, 32, 42 (permanent central canines), 13, 23, 33, 43 (permanent lateral canines), 14, 24, 34, 44 (permanent first premolars), 15, 25, 35, 45 (permanent second premolars), 16, 26, 36, 46 (permanent first molars), 17, 27, 37, 47 (permanent second molars).

**EEND.xx** upper limit of the emergence (in years of age) of the permanent tooth xx. NA if the emergence was right-censored.

xx takes values as for the variable EBEG. xx.

**FBEG.xx** lower limit for the caries time (in years of age, 'F' stands for 'failure') of the permanent tooth xx. NA if the caries time was left-censored.

xx takes values as for the variable EBEG. xx.

**FEND.xx** upper limit for the caries time (in years of age, 'F' stands for 'failure') of the permanent tooth xx. NA if the caries time was right-censored.

xx takes values as for the variable EBEG. xx.

Unfortunately, for all teeth except 16, 26, 36 and 46 almost all the caries times are right-censored. For teeth 16, 26, 36, 46, the amount of right-censoring is only about 25%.

**Txx.DMF** indicator whether a deciduous tooth xx was *decayed* or *missing due to caries* or *filled* on at most the last examination before the first examination when the emergence of the permanent successor was recorded.



xx takes values 53, 63, 73, 83 (deciduous lateral incisors), 54, 64, 74, 84 (deciduous first molars), 55, 65, 75, 85 (deciduous second molars).

**Txx.CAR** indicator whether a~deciduous tooth xx was removed due to the orthodontical reasons or decayed on at most the last examination before the first examination when the emergence of the permanent successor was recorded.

## Source

Biostatistical Centre, Katholieke Universiteit Leuven, Kapucijnenvoer 35, 3000 Leuven, Belgium

URL: <http://med.kuleuven.be/biostat/>

Data collection was supported by Unilever, Belgium. The Signal Tandmobiel project comprises the following partners: D. Declerck (Dental School, Catholic University Leuven), L. Martens (Dental School, University Ghent), J. Vanobbergen (Oral Health Promotion and Prevention, Flemish Dental Association), P. Bottenberg (Dental School, University Brussels), E. Lesaffre (Biostatistical Centre, Catholic University Leuven), K. Hoppenbrouwers (Youth Health Department, Catholic University Leuven; Flemish Association for Youth Health Care).

## References

Komárek, A., Lesaffre, E., Härkänen, T., Declerck, D., and Virtanen, J. I. (2005). A Bayesian analysis of multivariate doubly-interval-censored dental data. *Biostatistics*, **6**, 145–155.

Komárek, A. and Lesaffre, E. (2007). Bayesian accelerated failure time model for correlated interval-censored data with a normal mixture as an error distribution. *Statistica Sinica*, **17**, 549–569.

Lesaffre, E., Komárek, A., and Declerck, D. (2005). An overview of methods for interval-censored data with an emphasis on applications in dentistry. *Statistical Methods in Medical Research*, **14**, 539–552.

Vanobbergen, J., Martens, L., Lesaffre, E., and Declerck, D. (2000). The Signal-Tandmobiel project – a longitudinal intervention health promotion study in Flanders (Belgium): baseline and first year results. *European Journal of Paediatric Dentistry*, **2**, 87–96.

## See Also

[tandmob2](#)

## Examples

```
data(Tandmob)
summary(Tandmob)
```

TandmobEmer

*Signal Tandmobiel data - emergence times***Description**

This is a part of the [Tandmob](#) data containing only emergence times and some baseline covariates. Here, all left-censored emergence times have been changed into interval-censored with the lower limit of the intervals equal to 5 years of age (clinically minimal time before which the permanent teeth hardly emerge). Also censoring indicators are added to be able to use the data directly with the [NMixMCMC](#) function.

**IMPORTANT NOTICE:** It is possible to use these data for your research work under the condition that each manuscript is first approved by

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**Usage**

```
data(TandmobEmer)
```

**Format**

a data frame with 4 430 rows and the following variables

**IDNR** identification number of a child

**GENDER** character *boy* or *girl*

**GENDERNum** numeric, 0 = *boy*, 1 = *girl*

**DOB** character, date of birth in the format DDmmmYY

**PROVINCE** factor, code of the province with

**0** = Antwerpen

**1** = Vlaams Brabant

**2** = Limburg

**3** = Oost Vlaanderen

**4** = West Vlaanderen

**EDUC** factor, code of the educational system with

**0** = Free

**1** = Community school

**2** = Province/council school

**STARTBR** factor, code indicating the starting age of brushing the teeth (as reported by parents) with

- 1 = [0, 1] years
- 2 = (1, 2] years
- 3 = (2, 3] years
- 4 = (3, 4] years
- 5 = (4, 5] years
- 6 = later than at the age of 5

**EBEG.xx** lower limit of the emergence (in years of age) of the permanent tooth xx. It is equal to 5 if the emergence was originally left-censored.

xx takes values 11, 21, 31, 41 (permanent incisors), 12, 22, 32, 42 (permanent central canines), 13, 23, 33, 43 (permanent lateral canines), 14, 24, 34, 44 (permanent first premolars), 15, 25, 35, 45 (permanent second premolars), 16, 26, 36, 46 (permanent first molars), 17, 27, 37, 47 (permanent second molars).

**EEND.xx** upper limit of the emergence (in years of age) of the permanent tooth xx. NA if the emergence was right-censored.

xx takes values as for the variable EBEG . xx.

**CENSOR.xx** censoring indicator for the emergence. It is equal to 3 for interval-censored times and equal to 0 for right-censored times.

xx takes values as for the variable EBEG . xx.

### Source

Biostatistical Centre, Katholieke Universiteit Leuven, Kapucijnenvoer 35, 3000 Leuven, Belgium

URL: <http://med.kuleuven.be/biostat/>

Data collection was supported by Unilever, Belgium. The Signal Tandmobiel project comprises the following partners: D. Declerck (Dental School, Catholic University Leuven), L. Martens (Dental School, University Ghent), J. Vanobbergen (Oral Health Promotion and Prevention, Flemish Dental Association), P. Bottenberg (Dental School, University Brussels), E. Lesaffre (Biostatistical Centre, Catholic University Leuven), K. Hoppenbrouwers (Youth Health Department, Catholic University Leuven; Flemish Association for Youth Health Care).

### References

Komárek, A. (2009). A new R package for Bayesian estimation of multivariate normal mixtures allowing for selection of the number of components and interval-censored data. *Computational Statistics and Data Analysis*, **53**(12), 3932–3947.

Vanobbergen, J., Martens, L., Lesaffre, E., and Declerck, D. (2000). The Signal-Tandmobiel project – a longitudinal intervention health promotion study in Flanders (Belgium): baseline and first year results. *European Journal of Paediatric Dentistry*, **2**, 87-96.

### See Also

[Tandmob](#)

### Examples

```
data(TandmobEmer)
summary(TandmobEmer)
```

TMVN

*Truncated multivariate normal distribution***Description**

Random generation for the truncated multivariate normal distribution. The mean and covariance matrix of the original multivariate normal distribution are mean and Sigma. Truncation limits are given by a, b, type of truncation is given by trunc.

This function uses a Gibbs algorithm to produce a Markov chain whose stationary distribution is the targeted truncated multivariate normal distribution, see Geweke (1991) for more details. Be aware that the sampled values are not i.i.d.!

**Usage**

```
rTMVN(n, mean=c(0, 0), Sigma=diag(2), a, b, trunc, xinit)
```

**Arguments**

mean	a numeric vector of the mean of the original multivariate normal distribution.
Sigma	covariance matrix of the original multivariate normal distribution.
a	a numeric vector of the same length as mean of truncation limits 1.
b	a numeric vector of the same length as mean of truncation limits 2.
trunc	a numeric vector of the same length as mean describing the type of truncation in each margin. trunc=0 normal distribution is truncated on the interval $(a, \infty)$ .. Value of $b$ is ignored. trunc=1 degenerated normal distribution, all values are with probability 1 equal to $a$ , $b$ is ignored. trunc=2 normal distribution is truncated on the interval $(-\infty, a)$ . Value of $b$ is ignored. trunc=3 normal distribution is truncated on the interval $(a, b)$ . trunc=4 there is no truncation, values of $a$ and $b$ are ignored. If trunc is not given, it is assumed that it is equal to 4. Note that a, b and trunc must have the same length, with exception that b does not have to be supplied if all trunc values 0, 1, 2 or 4.
xinit	a numeric vector of the same length as mean with the initial value for the Gibbs sampler. If it is not supplied, the function determines itself the initial value.
n	number of observations to be sampled.

**Value**

A matrix with the sampled values (Markov chain) in rows.

**Author(s)**

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

**References**

Geweke, J. (1991). Efficient simulation from the multivariate normal and Student-t distributions subject to linear constraints and the evaluation of constraint probabilities. *Computer Sciences and Statistics*, **23**, 571–578.

**See Also**

[rTNorm](#).

**Examples**

```
## Not run:
set.seed(1977)

exam2 <- function(n, mu, sigma, rho, a, b, trunc)
{
  Sigma <- matrix(c(sigma[1]^2, rho*sigma[1]*sigma[2], rho*sigma[1]*sigma[2], sigma[2]^2), nrow=2)
  x <- rTMVN(n, mean=mu, Sigma=Sigma, a=a, b=b, trunc=trunc)
  x1.gr <- seq(mu[1]-3.5*sigma[1], mu[1]+3.5*sigma[1], length=100)
  x2.gr <- seq(mu[2]-3.5*sigma[2], mu[2]+3.5*sigma[2], length=100)
  z <- cbind(rep(x1.gr, 100), rep(x2.gr, each=100))
  dens.z <- matrix(dMVN(z, mean=mu, Sigma=Sigma), ncol=100)

  MEAN <- round(apply(x, 2, mean), 3)
  SIGMA <- var(x)
  SD <- sqrt(diag(SIGMA))
  RHO <- round(SIGMA[1,2]/(SD[1]*SD[2]), 3)
  SD <- round(SD, 3)

  layout(matrix(c(0,1,1,0, 2,2,3,3), nrow=2, byrow=TRUE))
  contour(x1.gr, x2.gr, dens.z, col="darkblue", xlab="x[1]", ylab="x[2]")
  points(x[,1], x[,2], col="red")
  title(sub=paste("Sample mean = ", MEAN[1], ", ", MEAN[2], ", Sample SD = ", SD[1], ", ", SD[2],
    ", Sample rho = ", RHO, sep=""))
  plot(1:n, x[,1], type="l", xlab="Iteration", ylab="x[1]", col="darkgreen")
  plot(1:n, x[,2], type="l", xlab="Iteration", ylab="x[2]", col="darkgreen")

  return(x)
}

x1 <- exam2(1000, mu=c(-1, 1), sigma=c(1, sqrt(2)), rho=0, a=c(-6, -9), b=c(4, 11), trunc=c(3, 3))
x2 <- exam2(1000, mu=c(-1, 1), sigma=c(1, sqrt(2)), rho=0.7, a=c(-6, -9), b=c(4, 11), trunc=c(3, 3))
x3 <- exam2(1000, mu=c(-1, 1), sigma=c(1, sqrt(2)), rho=0.7, a=c(-100, -100), b=c(100, 100),
  trunc=c(3, 3))
x4 <- exam2(1000, mu=c(-1, 1), sigma=c(1, sqrt(2)), rho=-0.7, a=c(-6, -9), b=c(4, 11),
  trunc=c(3, 3))
x5 <- exam2(1000, mu=c(-1, 1), sigma=c(1, sqrt(2)), rho=-0.9, a=c(-6, -9), b=c(4, 11),
  trunc=c(3, 3))
```

```

x6 <- exam2(1000, mu=c(-1, 1), sigma=c(1, sqrt(2)), rho=0.7, a=c(0, 0), trunc=c(0, 2))
x7 <- exam2(1000, mu=c(-1, 1), sigma=c(1, sqrt(2)), rho=0.7, a=c(-1, 1), trunc=c(0, 2))
x8 <- exam2(1000, mu=c(-1, 1), sigma=c(1, sqrt(2)), rho=0.7, a=c(-1, 1), trunc=c(1, 2))
x9 <- exam2(1000, mu=c(-1, 1), sigma=c(1, sqrt(2)), rho=0.7, a=c(-1.5, 0.5), b=c(-0.5, 1.5),
           trunc=c(3, 3))
x10 <- exam2(1000, mu=c(-1, 1), sigma=c(1, sqrt(2)), rho=0.7, a=c(-1.5, 0.5), b=c(-0.5, 1.5),
            trunc=c(4, 3))

## End(Not run)

```

TNorm

*Truncated normal distribution***Description**

Random generation for the truncated normal distribution. The mean and standard deviation of the original normal distribution are mean and sd. Truncation limits are given by a, b, type of truncation is given by trunc.

**Usage**

```
rTNorm(n, mean=0, sd=1, a, b, trunc)
```

**Arguments**

mean	mean (if common for all observations) or a vector of length n of means.
sd	standard deviation (if common for all observations) or a vector of length n of standard deviations. Note that mean and sd must have the same length, either 1 or n.
a	truncation limit 1 (if common for all observations) or a vector of length n of truncation limits 1.
b	truncation limit 2 (if common for all observations) or a vector of length n of truncation limits 2.
trunc	type of truncation (if common for all observations) or a vector of length n of types of truncation trunc= <b>0</b> normal distribution is truncated on the interval $(a, \infty)$ . Value of $b$ is ignored. trunc= <b>1</b> degenerated normal distribution, all values are with probability 1 equal to $a$ , $b$ is ignored. trunc= <b>2</b> normal distribution is truncated on the interval $(-\infty, a)$ . Value of $b$ is ignored. trunc= <b>3</b> normal distribution is truncated on the interval $(a, b)$ . trunc= <b>4</b> there is no truncation, values of $a$ and $b$ are ignored. If trunc is not given, it is assumed that it is equal to 4. Note that a, b and trunc must have the same length, either 1 or n with exception that b does not have to be supplied if trunc is 0, 1, 2 or 4.
n	number of observations to be sampled.

**Value**

A numeric vector with sampled values.

**Author(s)**

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

**References**

Geweke, J. (1991). Efficient simulation from the multivariate normal and Student-t distributions subject to linear constraints and the evaluation of constraint probabilities. *Computer Sciences and Statistics*, **23**, 571–578.

**See Also**

[rnorm](#), [rTMVN](#).

**Examples**

```
set.seed(1977)

### Not truncated normal distribution
x1 <- rTNorm(1000, mean=10, sd=3)
c(mean(x1), sd(x1), range(x1))

### Truncation from left only
x2 <- rTNorm(1000, mean=10, sd=3, a=7, trunc=0)
c(mean(x2), sd(x2), range(x2))

### Degenerated normal distribution
x6 <- rTNorm(1000, mean=10, sd=3, a=13, trunc=1)
c(mean(x6), sd(x6), range(x6))

### Truncation from right only
x3 <- rTNorm(1000, mean=10, sd=3, a=13, trunc=2)
c(mean(x3), sd(x3), range(x3))

### Truncation from both sides
x4 <- rTNorm(1000, mean=10, sd=3, a=7, b=13, trunc=3)
c(mean(x4), sd(x4), range(x4))

x5 <- rTNorm(1000, mean=10, sd=3, a=5.5, b=14.5, trunc=3)
c(mean(x5), sd(x5), range(x5))

oldPar <- par(mfrow=c(2, 3))
hist(x1, main="N(10, 3^2)")
hist(x2, main="TN(10, 3^2, 7, Infy)")
hist(x6, main="TN(10, 3^2, 13, 13)")
hist(x3, main="TN(10, 3^2, -Infy, 13)")
hist(x4, main="TN(10, 3^2, 7, 13)")
hist(x5, main="TN(10, 3^2, 5.5, 14.5)")
par(oldPar)
```

```

### Different truncation limits
n <- 1000
a <- rnorm(n, -2, 1)
b <- a + rgamma(n, 1, 1)
trunc <- rep(c(0, 1, 2, 3, 4), each=n/5)
x7 <- rTNorm(n, mean=1, sd=2, a=a, b=b, trunc=trunc)
cbind(trunc, a, x7)[1:10,]
sum(x7[1:(n/5)] > a[1:(n/5)])      ## must be equal to n/5

cbind(trunc, a, x7)[201:210,]
sum(x7[(n/5+1):(2*n/5)] == a[(n/5+1):(2*n/5)])      ## must be equal to n/5

cbind(trunc, x7, a)[401:410,]
sum(x7[(2*n/5+1):(3*n/5)] < a[(2*n/5+1):(3*n/5)])      ## must be equal to n/5

cbind(trunc, a, x7, b)[601:610,]
sum(x7[(3*n/5+1):(4*n/5)] > a[(3*n/5+1):(4*n/5)])      ## must be equal to n/5
sum(x7[(3*n/5+1):(4*n/5)] < b[(3*n/5+1):(4*n/5)])      ## must be equal to n/5

cbind(trunc, x7)[801:810,]

### Different moments and truncation limits
n <- 1000
mu <- rnorm(n, 1, 0.2)
sigma <- 0.5 + rgamma(n, 1, 1)
a <- rnorm(n, -2, 1)
b <- a + rgamma(n, 1, 1)
trunc <- rep(c(0, 1, 2, 3, 4), each=n/5)
x8 <- rTNorm(n, mean=1, sd=2, a=a, b=b, trunc=trunc)

### Truncation from left only
### (extreme cases when we truncate to the area
### where the original normal distribution has
### almost zero probability)
x2b <- rTNorm(1000, mean=0, sd=1, a=7.9, trunc=0)
c(mean(x2b), sd(x2b), range(x2b))

x2c <- rTNorm(1000, mean=1, sd=2, a=16, trunc=0)
c(mean(x2c), sd(x2c), range(x2c))

### Truncation from right only (extreme cases)
x3b <- rTNorm(1000, mean=0, sd=1, a=-7.9, trunc=2)
c(mean(x3b), sd(x3b), range(x3b))

x3c <- rTNorm(1000, mean=1, sd=2, a=-13, trunc=2)
c(mean(x3c), sd(x3c), range(x3c))

### Truncation from both sides (extreme cases)
x4b <- rTNorm(1000, mean=0, sd=1, a=-9, b=-7.9, trunc=3)
c(mean(x4b), sd(x4b), range(x4b))

x4c <- rTNorm(1000, mean=0, sd=1, a=7.9, b=9, trunc=3)

```



```
c(mean(x4c), sd(x4c), range(x4c))
```

---

tracePlots	<i>Traceplots for selected parameters</i>
------------	---

---

## Description

This function draws traceplots of selected parameters from the MCMC simulations ran using [NMixMCMC](#) or [GLMM\\_MCMC](#) functions.

## Usage

```
tracePlots(x, ...)

## Default S3 method:
tracePlots(x, ...)

## S3 method for class 'NMixMCMC'
tracePlots(x, param=c("Emix", "SDmix", "Cormix", "K", "w", "mu", "sd", "gammaInv"),
  relabel=FALSE, order,
  auto.layout=TRUE, xlab="Iteration", ylab, col="slateblue", main="", ...)

## S3 method for class 'NMixMCMClist'
tracePlots(x, param=c("Emix", "SDmix", "Cormix", "K", "w", "mu", "sd", "gammaInv"),
  relabel=FALSE,
  auto.layout=TRUE, xlab="Iteration", ylab, col=c("blue3", "red3"), main="", ...)

## S3 method for class 'GLMM_MCMC'
tracePlots(x, param=c("Deviance", "Cond.Deviance",
  "alpha", "Eb", "SDb", "Corb", "sigma_eps",
  "w_b", "mu_b", "sd_b", "gammaInv_b", "gammaInv_eps"),
  relabel=FALSE, order,
  auto.layout=TRUE, xlab="Iteration", ylab, col="slateblue", main="", ...)

## S3 method for class 'GLMM_MCMClist'
tracePlots(x, param=c("Deviance", "Cond.Deviance",
  "alpha", "Eb", "SDb", "Corb", "sigma_eps",
  "w_b", "mu_b", "sd_b", "gammaInv_b", "gammaInv_eps"),
  relabel=FALSE,
  auto.layout=TRUE, xlab="Iteration", ylab, col=c("blue3", "red3"), main="", ...)
```

## Arguments

**x** an object of appropriate class.

**param** a character string which specifies which sort of parameters is to be plotted.

**Emix** overall means (for each margin) of the normal mixture;

	<p><b>SDmix</b> overall standard deviations (for each margin) of the normal mixture;</p> <p><b>Cormix</b> overall correlations (each pair) of the normal mixture;</p> <p><b>K</b> number of mixture components;</p> <p><b>w, w_b</b> weights of each of mixture components. If <code>relabel</code> is <code>FALSE</code>, weights are not re-labeled before plotting;</p> <p><b>mu, mu_b</b> component means (each margin, each mixture component) of the normal mixture. The mixture means are shifted and scaled using <code>x\$scale\$shift</code> and <code>x\$scale\$scale</code> before plotting. If <code>relabel</code> is <code>FALSE</code>, means are not re-labeled before plotting;</p> <p><b>sd, sd_b</b> component standard deviations (each margin, each mixture component) of the normal mixture. The mixture standard deviations are scaled using <code>x\$scale\$scale</code> before plotting. If <code>relabel</code> is <code>FALSE</code>, standard deviations are not re-labeled before plotting;</p> <p><b>gammaInv, gammaInv_b, gammaInv_eps</b> variance hyperparameters;</p> <p><b>Deviance</b> deviance (marginal, with random effects integrated out) of the GLMM;</p> <p><b>Cond.Deviance</b> conditional deviance (given random effects) of the GLMM;</p> <p><b>alpha</b> fixed effects of the fitted GLMM;</p> <p><b>Eb</b> overall means (for each margin) of the random effects of the fitted GLMM;</p> <p><b>SDb</b> overall standard deviations (for each margin) of the random effects of the fitted GLMM;</p> <p><b>Corb</b> overall correlations (each pair) of the distribution of the random effects of the fitted GLMM.</p> <p><b>sigma_eps</b> standard deviations of the error terms in the (mixed) models for continuous responses.</p>
<code>relabel</code>	logical value. It indicates whether the chains with <code>param</code> being <code>w</code> , <code>mu</code> , <code>sd</code> , <code>w_b</code> , <code>mu_b</code> , <code>sd_b</code> should be re-labeled before plotting. Re-labelling is given by argument <code>order</code> . If <code>order</code> is missing then <code>x\$order</code> or <code>x\$order_b</code> determines re-labelling.
<code>order</code>	a matrix with $K$ columns and $M$ rows where $M$ is the length of MCMC. Each row of <code>order</code> must be a permutation of $(1, \dots, K)$ .
<code>auto.layout</code>	logical value. If <code>TRUE</code> , the plotting region is automatically divided to produce traceplots of all parameters. Note that <code>layout</code> must be set up automatically if there are more than 28 parameters to be plotted (often the case for correlations with <code>param</code> being <code>Corb</code> or for mixture means with <code>param</code> being <code>mu_b</code> ).
<code>xlab</code> , <code>ylab</code> , <code>col</code> , <code>main</code>	arguments passed to <code>plot</code> function. They all can be of length one (the value is used on all plots) or of length equal to the number of parameters to be plotted.
<code>...</code>	other arguments passed to <code>plot</code> function.

**Value**

invisible(x)

**Author(s)**

Arnošt Komárek &lt;arnost.komarek[AT]mff.cuni.cz&gt;

**See Also**

[NMixMCMC](#), [GLMM\\_MCMC](#), [NMixRelabel](#), [traceplot](#).

---

Wishart

*Wishart distribution*

---

**Description**

Wishart distribution

$$\text{Wishart}(\nu, \mathbf{S}),$$

where  $\nu$  are degrees of freedom of the Wishart distribution and  $\mathbf{S}$  is its scale matrix. The same parametrization as in Gelman (2004) is assumed, that is, if  $\mathbf{W} \sim \text{Wishart}(\nu, \mathbf{S})$  then

$$E(\mathbf{W}) = \nu\mathbf{S}.$$

Prior to version 3.4-1 of this package, functions `dWISHART` and `rWISHART` were called as `dWishart` and `rWishart`, respectively. The names were changed in order to avoid conflicts with `rWishart` from a standard package `stats`.

**Usage**

```
dWISHART(W, df, S, log=FALSE)
```

```
rWISHART(n, df, S)
```

**Arguments**

<code>W</code>	Either a matrix with the same number of rows and columns as <code>S</code> (1 point sampled from the Wishart distribution) or a matrix with <code>ncol</code> equal to <code>ncol*(ncol+1)/2</code> and <code>n</code> rows ( <code>n</code> points sampled from the Wishart distribution for which only lower triangles are given in rows of the matrix <code>W</code> ).
<code>n</code>	number of observations to be sampled.
<code>df</code>	degrees of freedom of the Wishart distribution.
<code>S</code>	scale matrix of the Wishart distribution.
<code>log</code>	logical; if <code>TRUE</code> , log-density is computed

**Details**

The density of the Wishart distribution is the following

$$f(\mathbf{W}) = \left( 2^{\nu p/2} \pi^{p(p-1)/4} \prod_{i=1}^p \Gamma\left(\frac{\nu+1-i}{2}\right) \right)^{-1} |\mathbf{S}|^{-\nu/2} |\mathbf{W}|^{(\nu-p-1)/2} \exp\left(-\frac{1}{2}\text{tr}(\mathbf{S}^{-1}\mathbf{W})\right),$$

where  $p$  is number of rows and columns of the matrix  $\mathbf{W}$ .

In the univariate case,  $\text{Wishart}(\nu, S)$  is the same as  $\text{Gamma}(\nu/2, 1/(2S))$ .

Generation of random numbers is performed by the algorithm described in Ripley (1987, pp. 99).

**Value**

Some objects.

**Value for dWISHART**

A numeric vector with evaluated (log-)density.

**Value for rWISHART**

If  $n$  equals 1 then a sampled symmetric matrix  $W$  is returned.

If  $n > 1$  then a matrix with sampled points (lower triangles of  $W$ ) in rows is returned.

**Author(s)**

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

**References**

Gelman, A., Carlin, J. B., Stern, H. S., and Rubin, D. B. (2004). *Bayesian Data Analysis, Second edition*. Boca Raton: Chapman and Hall/CRC.

Ripley, B. D. (1987). *Stochastic Simulation*. New York: John Wiley and Sons.

**See Also**

[rWishart](#).

**Examples**

```
set.seed(1977)
### The same as gamma(shape=df/2, rate=1/(2*S))
df <- 1
S <- 3

w <- rWISHART(n=1000, df=df, S=S)
mean(w)    ## should be close to df*S
var(w)     ## should be close to 2*df*S^2

dWISHART(w[1], df=df, S=S)
dWISHART(w[1], df=df, S=S, log=TRUE)

dens.w <- dWISHART(w, df=df, S=S)
dens.wG <- dgamma(w, shape=df/2, rate=1/(2*S))
rbind(dens.w[1:10], dens.wG[1:10])

ldens.w <- dWISHART(w, df=df, S=S, log=TRUE)
ldens.wG <- dgamma(w, shape=df/2, rate=1/(2*S), log=TRUE)
rbind(ldens.w[1:10], ldens.wG[1:10])

### Bivariate Wishart
```

```

df <- 2
S <- matrix(c(1,3,3,13), nrow=2)

print(w2a <- rWISHART(n=1, df=df, S=S))
dWISHART(w2a, df=df, S=S)

w2 <- rWISHART(n=1000, df=df, S=S)
print(w2[1:10,])
apply(w2, 2, mean)          ## should be close to df*S
(df*S)[lower.tri(S, diag=TRUE)]

dens.w2 <- dWISHART(w2, df=df, S=S)
ldens.w2 <- dWISHART(w2, df=df, S=S, log=TRUE)
cbind(w2[1:10,], data.frame(Density=dens.w2[1:10], Log.Density=ldens.w2[1:10]))

### Trivariate Wishart
df <- 3.5
S <- matrix(c(1,2,3,2,20,26,3,26,70), nrow=3)

print(w3a <- rWISHART(n=1, df=df, S=S))
dWISHART(w3a, df=df, S=S)

w3 <- rWISHART(n=1000, df=df, S=S)
print(w3[1:10,])
apply(w3, 2, mean)          ## should be close to df*S
(df*S)[lower.tri(S, diag=TRUE)]

dens.w3 <- dWISHART(w3, df=df, S=S)
ldens.w3 <- dWISHART(w3, df=df, S=S, log=TRUE)
cbind(w3[1:10,], data.frame(Density=dens.w3[1:10], Log.Density=ldens.w3[1:10]))

```

---

Y2T

---

*Transform fitted distribution of  $Y = \text{trans}(T)$  into distribution of  $T$* 


---

## Description

This method transforms fitted distribution of  $Y = \text{trans}(T)$  into distribution of  $T$ . Default transformation is a logarithmic transformation where  $\text{trans}(t) = \log(t)$ ,  $\text{itrans}(y) = \exp(y)$ ,  $\text{dtrans}(t) = 1/t$ .

## Usage

```

Y2T(x, ...)

## S3 method for class 'NMixPredDensMarg'
Y2T(x, itrans=exp, dtrans=function(x){return(1 / x)}, ...)

## S3 method for class 'NMixPlugDensMarg'
Y2T(x, itrans=exp, dtrans=function(x){return(1 / x)}, ...)

```

```
## S3 method for class 'NMixPredCDFMarg'
Y2T(x, itrans=exp, ...)

## S3 method for class 'NMixPredDensJoint2'
Y2T(x, itrans=exp, dtrans=function(x){return(1 / x)}, ...)

## S3 method for class 'NMixPlugDensJoint2'
Y2T(x, itrans=exp, dtrans=function(x){return(1 / x)}, ...)

## S3 method for class 'NMixPredCondDensMarg'
Y2T(x, itrans=exp, dtrans=function(x){return(1 / x)}, ...)

## S3 method for class 'NMixPlugCondDensMarg'
Y2T(x, itrans=exp, dtrans=function(x){return(1 / x)}, ...)

## S3 method for class 'NMixPredCondCDFMarg'
Y2T(x, itrans=exp, dtrans=function(x){return(1 / x)}, ...)

## S3 method for class 'NMixPredCondDensJoint2'
Y2T(x, itrans=exp, dtrans=function(x){return(1 / x)}, ...)

## S3 method for class 'NMixPlugCondDensJoint2'
Y2T(x, itrans=exp, dtrans=function(x){return(1 / x)}, ...)
```

### Arguments

<code>x</code>	an object of appropriate class.
<code>itrans</code>	either an object of class function or a list of objects of class function giving inverse transformations for each margin. If <code>itrans</code> is a single function then it is assumed that all margins were transformed in the same way.
<code>dtrans</code>	either an object of class function or a list of objects of class function giving derivatives of transformations for each margin. If <code>dtrans</code> is a single function then it is assumed that all margins were transformed in the same way.
<code>...</code>	optional additional arguments.

### Value

An object of the same class as argument `x`.

### Author(s)

Arnošt Komárek <arnost.komarek[AT]mff.cuni.cz>

### See Also

[NMixPredDensMarg](#), [NMixPlugDensMarg](#), [NMixPredCDFMarg](#), [NMixPredDensJoint2](#), [NMixPlugDensJoint2](#), [NMixPredCondDensMarg](#), [NMixPlugCondDensMarg](#), [NMixPredCondCDFMarg](#), [NMixPredCondDensJoint2](#), [NMixPlugCondDensJoint2](#).

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