# Package 'mixtools'

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# Description

Performs a parametric bootstrap by producing B bootstrap realizations of the likelihood ratio statistic for testing the null hypothesis of a k-component fit versus the alternative hypothesis of a (k+1)-component fit to various mixture models. This is performed for up to a specified number of maximum components, k. A p-value is calculated for each test and once the p-value is above a specified significance level, the testing terminates. An optional histogram showing the distribution of the likelihood ratio statistic along with the observed statistic can also be produced.

# Usage

```
boot.comp(y, x = NULL, N = NULL, max.comp = 2, B = 100,
    sig = 0.05, arbmean = TRUE, arbvar = TRUE,
    mix.type = c("logisregmix", "multmix", "mvnormalmix",
        "normalmix", "poisregmix", "regmix", "regmix.mixed",
        "repnormmix"), hist = TRUE, ...)
```

able.

# **Arguments**

У	The raw data for multmix, mvnormalmix, normalmix, and repnormmix and the response values for logisregmix, poisregmix, and regmix. See the documentation concerning their respective EM algorithms for specific structure of the raw data.
x	The predictor values required only for the regression mixtures logisregmix, poisregmix, and regmix. A column of 1s for the intercept term must not be included! See the documentation concerning their respective EM algorithms for specific structure of the predictor values.
N	An n-vector of number of trials for the logistic regression type logisregmix. If NULL, then N is an n-vector of 1s for binary logistic regression.
max.comp	The maximum number of components to test for. The default is 2. This function will perform a test of k-components versus $(k+1)$ -components sequentially until we fail to reject the null hypothesis. This decision rule is governed by the calculated p-value and sig.
В	The number of bootstrap realizations of the likelihood ratio statistic to produce. The default is 100, but ideally, values of 1000 or more would be more accept-

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The significance level for which to compare the p-value against when perform-

ing the test of k-components versus (k+1)-components.

arbmean If FALSE, then a scale mixture analysis can be performed for mvnormalmix,

normalmix, regmix, or repnormmix. The default is TRUE.

arbvar If FALSE, then a location mixture analysis can be performed for mvnormalmix,

normalmix, regmix, or repnormmix. The default is TRUE.

mix.type The type of mixture analysis you wish to perform. The data inputted for y and

x depend on which type of mixture is selected. logisregmix corresponds to a mixture of logistic regressions. multmix corresponds to a mixture of multinomials with data determined by the cut-point method. mvnormalmix corresponds to a mixture of multivariate normals. normalmix corresponds to a mixture of univariate normals. poisregmix corresponds to a mixture of Poisson regressions. regmix corresponds to a mixture of regressions with normal components. regmix.mixed corresponds to a mixture of regressions with random or mixed effects. repnormmix corresponds to a mixture of normals with repeated mea-

surements.

hist An argument to provide a matrix plot of histograms for the boostrapped likeli-

hood ratio statistic.

... Additional arguments passed to the various EM algorithms for the mixture of

interest.

#### Value

boot.comp returns a list with items:

p. values The p-values for each test of k-components versus (k+1)-components.

log.lik The B bootstrap realizations of the likelihood ratio statistic.

obs.log.lik The observed likelihood ratio statistic for each test which is used in determining

the p-values.

#### References

McLachlan, G. J. and Peel, D. (2000) Finite Mixture Models, John Wiley & Sons, Inc.

### See Also

logis regmix EM, multmix EM, mvnormal mix EM, normal mix EM, pois regmix EM, regmix EM, regmix EM, mix ed, repnormmix EM

# Examples

```
## Bootstrapping to test the number of components on the RTdata.
```

```
data(RTdata)
set.seed(100)
x <- as.matrix(RTdata[, 1:3])
y <- makemultdata(x, cuts = quantile(x, (1:9)/10))$y
a <- boot.comp(y = y, max.comp = 1, B = 5, mix.type = "multmix",</pre>
```

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```
epsilon = 1e-3) a$p.values
```

boot.se

Performs Parametric Bootstrap for Standard Error Approximation

# Description

Performs a parametric bootstrap by producing B bootstrap samples for the parameters in the specified mixture model.

# Usage

```
boot.se(em.fit, B = 100, arbmean = TRUE, arbvar = TRUE, N = NULL, \ldots)
```

# **Arguments**

em.fit	An object of class mixEM. The estimates produced in em.fit will be used as the parameters for the distribution from which we generate the bootstrap data.
В	The number of bootstrap samples to produce. The default is 100, but ideally, values of 1000 or more would be more acceptable.
arbmean	If FALSE, then a scale mixture analysis can be performed for mvnormalmix, normalmix, regmix, or repnormmix. The default is TRUE.
arbvar	If FALSE, then a location mixture analysis can be performed for mvnormalmix, normalmix, regmix, or repnormmix. The default is TRUE.
N	An n-vector of number of trials for the logistic regression type logisregmix. If NULL, then N is an n-vector of 1s for binary logistic regression.
•••	Additional arguments passed to the various EM algorithms for the mixture of interest.

# Value

boot. se returns a list with the bootstrap samples and standard errors for the mixture of interest.

# References

McLachlan, G. J. and Peel, D. (2000) Finite Mixture Models, John Wiley \& Sons, Inc.

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### **Examples**

```
## Bootstrapping standard errors for a regression mixture case.

data(NOdata)
attach(NOdata)
set.seed(100)
em.out <- regmixEM(Equivalence, NO, arbvar = FALSE)
out.bs <- boot.se(em.out, B = 10, arbvar = FALSE)
out.bs</pre>
```

CO2data

GNP and CO2 Data Set

# **Description**

This data set gives the gross national product (GNP) per capita in 1996 for various countries as well as their estimated carbon dioxide (CO2) emission per capita for the same year.

# Usage

CO2data

### **Format**

This data frame consists of 28 countries and the following columns:

- GNPThe gross national product per capita in 1996.
- CO2The estimated carbon dioxide emission per capita in 1996.
- countryAn abbreviation pertaining to the country measured (e.g., "GRC" = Greece and "CH" = Switzerland).

### References

Hurn, M., Justel, A. and Robert, C. P. (2003) Estimating Mixtures of Regressions, *Journal of Computational and Graphical Statistics* **12(1)**, 55–79.

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compCDF	Plot the Component CDF	

# Description

Plot the components' CDF via the posterior probabilities.

### Usage

### **Arguments**

data	A matrix containing the raw data. Rows are subjects and columns are repeated measurements.
weights	The weights to compute the empirical CDF; however, most of time they are the posterior probabilities.
x	The points at which the CDFs are to be evaluated.
comp	The mixture components for which CDFs are desired.
makeplot	Logical: Should a plot be produced as a side effect?
	Additional arguments (other than 1ty and type, which are already used) to be passed directly to plot and lines functions.

### **Details**

When makeplot is TRUE, a line plot is produced of the CDFs evaluated at x. The plot is not a step function plot; the points (x, CDF(x)) are simply joined by line segments.

#### Value

A matrix with length(comp) rows and length(x) columns in which each row gives the CDF evaluated at each point of x.

### References

McLachlan, G. J. and Peel, D. (2000) Finite Mixture Models, John Wiley & Sons, Inc.

Elmore, R. T., Hettmansperger, T. P. and Xuan, F. (2004) The Sign Statistic, One-Way Layouts and Mixture Models, *Statistical Science* **19(4)**, 579–587.

#### See Also

```
makemultdata, multmixmodel.sel, multmixEM.
```

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### **Examples**

density.npEM

Normal kernel density estimate for nonparametric EM output

# **Description**

Takes an object of class npEM and returns an object of class density giving the kernel density estimate for the selected component and, if applicable, the selected block.

# Usage

```
## S3 method for class 'npEM'
density(x, u=NULL, component=1, block=1, scale=FALSE, ...)
```

### **Arguments**

X	An object of class npEM such as the output of the npEM or spEMsymloc functions.
u	Vector of points at which the density is to be evaluated
component	Mixture component number; should be an integer from 1 to the number of columns of x\$posteriors.
block	Block of repeated measures. Only applicable in repeated measures case, for which x\$blockid exists; should be an integer from 1 to max(x\$blockid).
scale	Logical: If TRUE, multiply the density values by the corresponding mixing proportions found in $x$ 1ambdahat
	Additional arguments; not used by this method.

### **Details**

The bandwidth is taken to be the same as that used to produce the npEM object, which is given by x\$bandwidth.

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### Value

density.npEM returns a list of type "density". See density for details. In particular, the output of density.npEM may be used directly by functions such as plot or lines.

### See Also

```
npEM, spEMsymloc, plot.npEM
```

### **Examples**

```
## Look at histogram of Old Faithful waiting times
data(faithful)
Minutes <- faithful$waiting
hist(Minutes, freq=FALSE)
## Superimpose equal-variance normal mixture fit:
set.seed(100)
nm <- normalmixEM(Minutes, mu=c(50,80), sigma=5, arbvar=FALSE, fast=TRUE)</pre>
x <- seq(min(Minutes), max(Minutes), len=200)</pre>
for (j in 1:2)
  lines(x, nm$lambda[j]*dnorm(x, mean=nm$mu[j], sd=nm$sigma), lwd=3, lty=2)
## Superimpose several semiparametric fits with different bandwidths:
bw <- c(1, 3, 5)
for (i in 1:3) {
  sp <- spEMsymloc(Minutes, c(50,80), bw=bw[i])</pre>
  for (j in 1:2)
    lines(density(sp, component=j, scale=TRUE), col=1+i, lwd=2)
}
legend("topleft", legend=paste("Bandwidth =",bw), fill=2:4)
```

density.spEM

Normal kernel density estimate for semiparametric EM output

# **Description**

Takes an object of class spEM and returns an object of class density giving the kernel density estimate.

### Usage

```
## S3 method for class 'spEM'
density(x, u=NULL, component=1, block=1, scale=FALSE, ...)
```

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### **Arguments**

X	An object of class npEM such as the output of the npEM or spEMsym1oc functions.
u	Vector of points at which the density is to be evaluated
component	Mixture component number; should be an integer from 1 to the number of columns of $x$ -posteriors.
block	Block of repeated measures. Only applicable in repeated measures case, for which x\$blockid exists; should be an integer from 1 to max(x\$blockid).
scale	Logical: If TRUE, multiply the density values by the corresponding mixing proportions found in $x$ 1ambdahat
	Additional arguments; not used by this method.

### **Details**

The bandwidth is taken to be the same as that used to produce the npEM object, which is given by x\$bandwidth.

### Value

density.spEM returns a list of type "density". See density for details. In particular, the output of density.spEM may be used directly by functions such as plot or lines.

### See Also

```
spEM, spEMsymloc, plot.spEM
```

### **Examples**

depth

Elliptical and Spherical Depth

# **Description**

Computation of spherical or elliptical depth.

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# Usage

```
depth(pts, x, Cx = var(x))
```

# **Arguments**

pts	A kxd matrix containing the k points that one wants to compute the depth. Each row is a point.
x	A nxd matrix containing the reference data. Each row is an observation.
Сх	A dxd scatter matrix for the data x where the default is $var(x)$ . When $Cx = I(d)$ , it returns the sphercial depth.

### Value

depth returns a k-vector where each entry is the elliptical depth of a point in pts.

### Note

depth is used in regcr.

#### References

Elmore, R. T., Hettmansperger, T. P. and Xuan, F. (2000) Spherical Data Depth and a Multivariate Median, *Proceedings of Data Depth: Robust Multivariate Statistical Analysis, Computational Geometry and Applications*.

### See Also

regcr

# Examples

```
set.seed(100)
x <- matrix(rnorm(200),nc = 2)
depth(x[1:3, ], x)</pre>
```

dmvnorm

The Multivariate Normal Density

# **Description**

Density and log-density for the multivariate normal distribution with mean equal to mu and variance matrix equal to sigma.

# Usage

```
dmvnorm(y, mu=NULL, sigma=NULL)
logdmvnorm(y, mu=NULL, sigma=NULL)
```

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# **Arguments**

У	Either a $d$ - vector or an $n \times d$ matrix, where $d$ is the dimension of the normal
	distribution and $n$ is the number of points at which the density is to be evaluated.
mu	$\boldsymbol{d}$ - vector: Mean of the normal distribution (or NULL uses the origin as default)
sigma	This $d \times d$ matrix is the variance matrix of the normal distribution (or NULL
	uses the identity matrix as default)

# **Details**

This code is written to be efficient, using the qr-decomposition of the covariance matrix (and using it only once, rather than recalculating it for both the determinant and the inverse of sigma).

# Value

dmvnorm gives the densities, while logdmvnorm gives the logarithm of the densities.

### See Also

```
qr, qr.solve, dnorm, rmvnorm
```

ellipse

Draw Two-Dimensional Ellipse Based on Mean and Covariance

# **Description**

Draw a two-dimensional ellipse that traces a bivariate normal density contour for a given mean vector, covariance matrix, and probability content.

# Usage

# **Arguments**

mu	A 2-vector giving the mean.
sigma	A 2x2 matrix giving the covariance matrix.
alpha	Probability to be excluded from the ellipse. The default value is alpha = $.05$ , which results in a $95\%$ ellipse.
npoints	Number of points comprising the border of the ellipse.
newplot	If newplot = TRUE and draw = TRUE, plot the ellipse on a new plot. If newplot = FALSE and draw = TRUE, add the ellipse to an existing plot.
draw	If TRUE, draw the ellipse.
	Graphical parameters passed to lines or plot command.

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# Value

ellipse returns an npointsx2 matrix of the points forming the border of the ellipse.

#### References

Johnson, R. A. and Wichern, D. W. (2002) *Applied Multivariate Statistical Analysis, Fifth Edition*, Prentice Hall.

### See Also

regcr

### **Examples**

```
## Produce a 95% ellipse with the specified mean and covariance structure. 
 mu \leftarrow c(1, 3) sigma \leftarrow matrix(c(1, .3, .3, 1.5), 2, 2) ellipse(mu, sigma, npoints = 200, newplot = TRUE)
```

flaremixEM

EM Algorithm for Mixtures of Regressions with Flare

# Description

Returns output for 2-component mixture of regressions with flaring using an EM algorithm with one step of Newton-Raphson requiring an adaptive barrier for maximization of the objective function. A mixture of regressions with flare occurs when there appears to be a common regression relationship for the data, but the error terms have a mixture structure of one normal component and one exponential component.

# Usage

# Arguments

У	An n-vector of response values.
X	An n-vector of predictor values. An intercept term will be added by default.
lambda	Initial value of mixing proportions. Entries should sum to 1.
beta	Initial value of beta parameters. Should be a $2x2$ matrix where the columns correspond to the component.
sigma	A vector of standard deviations.

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A scalar for the exponential component's rate. alpha

A vector specifying the barrier constants to use. The first barrier constant where nu

the algorithm converges is used.

The convergence criterion. epsilon

The maximum number of iterations. maxit

verb If TRUE, then various updates are printed during each iteration of the algorithm. restart

The number of times to restart the algorithm in case convergence is not attained.

The default is 50.

### Value

flaremixEM returns a list of class mixEM with items:

The set of predictors (which includes a column of 1's). Х

y The response values.

posterior An nx2 matrix of posterior probabilities for observations.

The final mixing proportions. lambda beta The final regression coefficients. The final standard deviations. sigma alpha The final exponential rate.

loglik The final log-likelihood.

all.loglik A vector of each iteration's log-likelihood.

ft A character vector giving the name of the function.

# See Also

### regmixEM

# Examples

```
## Simulation output.
set.seed(100)
j=1
while(j == 1){
   x1 <- runif(30, 0, 10)
   x2 <- runif(20, 10, 20)
   x3 <- runif(30, 20, 30)
   y1 <- 3+4*x1+rnorm(30, sd = 1)
   y2 < -3+4*x2+rexp(20, rate = .05)
   y3 < -3+4*x3+rnorm(30, sd = 1)
    x < -c(x1, x2, x3)
   y < -c(y1, y2, y3)
   nu <- (1:30)/2
   out <- try(flaremixEM(y, x, beta = c(3, 4), nu = nu,
               lambda = c(.75, .25), sigma = 1), silent = TRUE)
```

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```
if(class(out) == "try-error"){
        j <- 1
    } else j <- 2
}

out[4:7]
plot(x, y, pch = 19)
abline(out$beta)</pre>
```

 ${\tt gammamixEM}$ 

EM Algorithm for Mixtures of Gamma Distributions

# Description

Return EM algorithm output for mixtures of gamma distributions.

# Usage

```
gammamixEM(x, lambda = NULL, alpha = NULL, beta = NULL, k = 2, epsilon = 1e-08, maxit = 1000, maxrestarts=20, verb = FALSE)
```

# **Arguments**

Х	A vector of length n consisting of the data.
lambda	Initial value of mixing proportions. If NULL, then lambda is random from a uniform Dirichlet distribution (i.e., its entries are uniform random and then it is normalized to sum to 1).
alpha	Starting value of vector of component shape parameters. If non-NULL and a vector, k is set to length(alpha). If NULL, then the initial value is estimated by partitioning the data into k regions (with lambda determining the proportion of values in each region) and then calculating the method of moments estimates.
beta	Starting value of vector of component scale parameters. If non-NULL and a vector, k is set to length(beta). If NULL, then the initial value is estimated the same method described for alpha.
k	Number of components. Initial value ignored unless alpha and beta are both NULL.
epsilon	The convergence criterion. Convergence is declared when the change in the observed data log-likelihood increases by less than epsilon.
maxit	The maximum number of iterations.
maxrestarts	The maximum number of restarts allowed in case of a problem with the particular starting values chosen (each restart uses randomly chosen starting values).
verb	If TRUE, then various updates are printed during each iteration of the algorithm.

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### Value

gammamixEM returns a list of class mixEM with items:

x The raw data.

lambda The final mixing proportions.

gamma.pars A 2xk matrix where each column provides the component estimates of alpha

and beta.

loglik The final log-likelihood.

posterior An nxk matrix of posterior probabilities for observations.

all.loglik A vector of each iteration's log-likelihood. This vector includes both the initial

and the final values; thus, the number of iterations is one less than its length.

ft A character vector giving the name of the function.

### References

Dempster, A. P., Laird, N. M., and Rubin, D. B. (1977) Maximum Likelihood From Incomplete Data Via the EM Algorithm, *Journal of the Royal Statistical Society, Series B*, **39**(1), 1–38.

### **Examples**

```
##Analyzing a 3-component mixture of gammas.
set.seed(100)
x <- c(rgamma(200, shape = 0.2, scale = 14), rgamma(200, shape = 32, scale = 10), rgamma(200, shape = 5, scale = 6))
out <- gammamixEM(x, lambda = c(1, 1, 1)/3, verb = TRUE)
out[2:4]</pre>
```

Habituationdata

Infant habituation data

# **Description**

From Thomas et al (2011):

"Habituation is a standard method of studying infant behaviors. Indeed, much of what is known about infant memory and perception rests on habituation methods. Six-month infants (n = 51) were habituated to a checker-board pattern on two occasions, one week apart. On each occasion, the infant was presented with the checkerboard pattern and the length of time the infant viewed the pattern before disengaging was recorded; this denoted the end of a trial. After disengagement, another trial was presented. The procedure was implemented for eleven trials. The conventional index of habituation performance is the summed observed fixation to the checkerboard pattern over the eleven trials. Thus, an index of reliability focuses on how these fixation times, in seconds, on the two assessment occasions correlate: r = .29."

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### Usage

```
data(Habituationdata)
```

#### **Format**

A data frame with two variables, m1 and m2, and 51 cases. The two variables are the summed observations times for the two occasions described above.

### Author(s)

Hoben Thomas

#### Source

Original source: Thomas et al. (2011). See references section.

# References

Thomas, H., Lohaus, A., and Domsch, H. (2011), Extensions of Reliability Theory, in Nonparametric Statistics and Mixture Models: A Festschrift in Honor of Thomas Hettmansperger (Singapore: World Scientific), pp. 309-316.

hmeEM

EM Algorithm for Mixtures-of-Experts

# **Description**

Returns EM algorithm output for a mixture-of-experts model. Currently, this code only handles a 2-component mixture-of-experts, but will be extended to the general k-component hierarchical mixture-of-experts.

# Usage

```
hmeEM(y, x, lambda = NULL, beta = NULL, sigma = NULL, w = NULL,
    k = 2, addintercept = TRUE, epsilon = 1e-08,
    maxit = 10000, verb = FALSE)
```

### **Arguments**

١	,	An n-vector	of	response	values.

x An nxp matrix of predictors. See addintercept below.

lambda Initial value of mixing proportions, which are modeled as an inverse logit func-

tion of the predictors. Entries should sum to 1. If NULL, then lambda is taken

as 1/k for each x.

beta Initial value of beta parameters. Should be a pxk matrix, where p is the num-

ber of columns of x and k is number of components. If NULL, then beta has

standard normal entries according to a binning method done on the data.

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sigma A vector of standard deviations. If NULL, then  $1/\text{sigma}^2$  has random standard

exponential entries according to a binning method done on the data.

w A p-vector of coefficients for the way the mixing proportions are modeled. See

lambda.

k Number of components. Currently, only k=2 is accepted.

addintercept If TRUE, a column of ones is appended to the x matrix before the value of p is

calculated.

epsilon The convergence criterion.

maxit The maximum number of iterations.

verb If TRUE, then various updates are printed during each iteration of the algorithm.

#### Value

hmeEM returns a list of class mixEM with items:

x The set of predictors (which includes a column of 1's if addintercept = TRUE).

y The response values.

W The final coefficients for the functional form of the mixing proportions.

lambda An nxk matrix of the final mixing proportions.

beta The final regression coefficients.

sigma The final standard deviations. If arbmean = FALSE, then only the smallest stan-

dard deviation is returned. See scale below.

loglik The final log-likelihood.

posterior An nxk matrix of posterior probabilities for observations.

all.loglik A vector of each iteration's log-likelihood.

restarts The number of times the algorithm restarted due to unacceptable choice of initial

values.

ft A character vector giving the name of the function.

#### References

Jacobs, R. A., Jordan, M. I., Nowlan, S. J. and Hinton, G. E. (1991) Adaptive Mixtures of Local Experts, *Neural Computation* **3(1)**, 79–87.

McLachlan, G. J. and Peel, D. (2000) Finite Mixture Models, John Wiley & Sons, Inc.

### See Also

regmixEM

ise.npEM

### **Examples**

```
## EM output for NOdata.

data(NOdata)
attach(NOdata)
set.seed(100)
em.out <- regmixEM(Equivalence, NO)
hme.out <- hmeEM(Equivalence, NO, beta = em.out$beta)
hme.out[3:7]</pre>
```

ise.npEM

Integrated Squared Error for a selected density from npEM output

# Description

Computes the integrated squared error for a selected estimated density from npEM output (selected by specifying the component and block number), relative to a true pdf that must be specified by the user. The range for the numerical integration must be specified. This function also returns (by default) a plot of the true and estimated densities.

### Usage

### **Arguments**

npEMout An object of class npEM such as the output of the npEM function

component, block

Component and block of particular density to analyze from npEMout.

truepdf an R function taking a numeric first argument and returning a numeric vector of

the same length. Returning a non-finite element will generate an error.

lower, upper the limits of integration. Can be infinite.

plots logical: Should plots be produced?

... additional arguments to be passed to truepdf (and that may be mandatory like,

e.g., the df = argument of dt). Remember to use argument names not matching

those of ise.npRM.

### **Details**

This function calls the wkde (weighted kernel density estimate) function.

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#### Value

Just as for the integrate function, a list of class "integrate" with components

value the final estimate of the integral.

abs.error estimate of the modulus of the absolute error.

subdivisions the number of subintervals produced in the subdivision process.

message "OK" or a character string giving the error message.

call the matched call.

#### References

 Benaglia, T., Chauveau, D., and Hunter, D. R. (2009), An EM-like algorithm for semi- and non-parametric estimation in multivariate mixtures, Journal of Computational and Graphical Statistics, 18, 505-526.

• Benaglia, T., Chauveau, D., Hunter, D. R., and Young, D. (2009), mixtools: An R package for analyzing finite mixture models. Journal of Statistical Software, 32(6):1-29.

### See Also

```
npEM, wkde, integrate
```

### **Examples**

```
# Mixture with mv gaussian model
set.seed(100)
m < -2 \# no. of components
r < -3 \# no. of repeated measures (coordinates)
lambda <- c(0.4, 0.6)
# Note: Need first 2 coordinates conditionally iid due to block structure
mu \leftarrow matrix(c(0, 0, 0, 3, 3, 5), m, r, byrow=TRUE) # means
sigma <- matrix(rep(1, 6), m, r, byrow=TRUE) # stdevs</pre>
blockid = c(1,1,2) # block structure of coordinates
n <- 500
x <- rmvnormmix(n, lambda, mu, sigma) # simulated data
# fit the model with "arbitrary" initial centers
centers <- matrix(c(0, 0, 0, 4, 4, 4), 2, 3, byrow=TRUE)
a <- npEM(x, centers, blockid, eps=1e-8, verb=FALSE)
# Calculate integrated squared error for j=2, b=1:
j <- 2 # component</pre>
b <- 1 # block
coords <- a$blockid == b</pre>
ise.npEM(a, j, b, dnorm, lower=0, upper=10, plots=TRUE,
         mean=mu[j,coords][1], sd=sigma[j, coords][1])
# The following (lengthy) example recreates the normal multivariate
# mixture model simulation from Benaglia et al (2009).
mu \leftarrow matrix(c(0, 0, 0, 3, 4, 5), m, r, byrow=TRUE)
```

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```
nbrep <- 5 # Benaglia et al use 300 replications</pre>
# matrix for storing sums of Integrated Squared Errors
ISE <- matrix(0,m,r,dimnames=list(Components=1:m, Blocks=1:r))</pre>
nblabsw <- 0 # no. of label switches
for (mc in 1:nbrep) {
 print(paste("REPETITION", mc))
x \leftarrow rmvnormmix(n, lambda, mu, sigma) # simulated data
 a <- npEM(x, centers, verb=FALSE) #default:
if (a$lambda[1] > a$lambda[2]) nblabsw <- nblabsw + 1</pre>
for (j in 1:m) { # for each component
for (k in 1:r) { # for each coordinate; not assuming iid!
      # dnorm with correct mean, sd is the true density:
      ISE[j,k] \leftarrow ISE[j,k] + ise.npEM(a, j, k, dnorm, lower=mu[j,k]-5,
                upper=mu[j,k]+5, plots=FALSE, mean=mu[j,k],
                sd=sigma[j,k])$value
   }
MISE <- ISE/nbrep # Mean ISE
sqMISE <- sqrt(MISE) # root-mean-integrated-squared error</pre>
sqMISE
```

logisregmixEM

EM Algorithm for Mixtures of Logistic Regressions

### **Description**

Returns EM algorithm output for mixtures of logistic regressions with arbitrarily many components.

### Usage

### **Arguments**

٧	, A	An n-vector	of successes	out of N trials.

x An nxp matrix of predictors. See addintercept below.

N An n-vector of number of trials for the logistic regression. If NULL, then N is

an n-vector of 1s for binary logistic regression.

lambda Initial value of mixing proportions. Entries should sum to 1. This determines number of components. If NULL, then lambda is random from uniform Dirich-

let and number of components is determined by beta.

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beta Initial value of beta parameters. Should be a pxk matrix, where p is the num-

ber of columns of x and k is number of components. If NULL, then beta is generated by binning the data into k bins and using glm on the values in each of the bins. If both lambda and beta are NULL, then number of components is

determined by k.

k Number of components. Ignored unless lambda and beta are both NULL.

addintercept If TRUE, a column of ones is appended to the x matrix before the value of p is

calculated.

epsilon The convergence criterion.

maxit The maximum number of iterations.

verb If TRUE, then various updates are printed during each iteration of the algorithm.

#### Value

logisregmixEM returns a list of class mixEM with items:

x The predictor values. y The response values.

lambda The final mixing proportions.

beta The final logistic regression coefficients.

loglik The final log-likelihood.

posterior An nxk matrix of posterior probabilities for observations.

all.loglik A vector of each iteration's log-likelihood.

restarts The number of times the algorithm restarted due to unacceptable choice of initial

values.

ft A character vector giving the name of the function.

#### References

McLachlan, G. J. and Peel, D. (2000) Finite Mixture Models, John Wiley & Sons, Inc.

### See Also

```
poisregmixEM
```

### **Examples**

```
## EM output for data generated from a 2-component logistic regression model. set.seed(100) beta <- matrix(c(1, .5, 2, -.8), 2, 2) x <- runif(50, 0, 10) x1 <- cbind(1, x) xbeta <- x1\%*beta N <- ceiling(runif(50, 50, 75)) w <- rbinom(50, 1, .3)
```

 $y \leftarrow w*rbinom(50, size = N, prob = (1/(1+exp(-xbeta[, 1]))))+$ 

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```
(1-w)*rbinom(50, size = N, prob =
              (1/(1+exp(-xbeta[, 2]))))
out.1 <- logisregmixEM(y, x, N, verb = TRUE, epsilon = 1e-01)
out.1
## EM output for data generated from a 2-component binary logistic regression model.
beta <- matrix(c(-10, .1, 20, -.1), 2, 2)
x <- runif(500, 50, 250)
x1 \leftarrow cbind(1, x)
xbeta <- x1%*%beta
w < - rbinom(500, 1, .3)
y \leftarrow w*rbinom(500, size = 1, prob = (1/(1+exp(-xbeta[, 1]))))+
              (1-w)*rbinom(500, size = 1, prob =
              (1/(1+exp(-xbeta[, 2]))))
out.2 <- logisregmixEM(y, x, beta = beta, lambda = c(.3, .7),
                       verb = TRUE, epsilon = 1e-01)
out.2
```

makemultdata

Produce Cutpoint Multinomial Data

# Description

Change data into a matrix of multinomial counts using the cutpoint method and generate EM algorithm starting values for a k-component mixture of multinomials.

#### Usage

```
makemultdata(..., cuts)
```

### **Arguments**

. . .

Either vectors (possibly of different lengths) of raw data or an nxm matrix (or data frame) of data. If ... are vectors of varying length, then makemultdata will create a matrix of size nxm where n is the sample size and m is the length of the vector with maximum length. Those vectors with length less than m will have NAs to make the corresponding row in the matrix of length m. If ... is a matrix (or data frame), then the rows must correspond to the sample and the columns the repeated measures.

cuts

A vector of cutpoints. This vector is sorted by the algorithm.

#### **Details**

The (i, j)th entry of the matrix y (for j < p) is equal to the number of entries in the ith column of x that are less than or equal to cuts[j]. The (i, p)th entry is equal to the number of entries greater than cuts[j].

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### Value

makemultdata returns an object which is a list with components:

x An nxm matrix of the raw data.

y An nxp matrix of the discretized data where p is one more than the number of cutpoints. Each row is a multinomial vector of counts. In particular, each row should sum to the number of repeated measures for that sample.

#### References

Elmore, R. T., Hettmansperger, T. P. and Xuan, F. (2004) The Sign Statistic, One-Way Layouts and Mixture Models, *Statistical Science* **19(4)**, 579–587.

### See Also

```
compCDF, multmixmodel.sel, multmixEM
```

#### **Examples**

```
## Randomly generated data.
set.seed(100)
y <- matrix(rpois(70, 6), 10, 7)
cuts <- c(2, 5, 7)
out1 <- makemultdata(y, cuts = cuts)</pre>
out1
## The sulfur content of the coal seams in Texas.
A \leftarrow c(1.51, 1.92, 1.08, 2.04, 2.14, 1.76, 1.17)
B \leftarrow c(1.69, 0.64, .9, 1.41, 1.01, .84, 1.28, 1.59)
C \leftarrow c(1.56, 1.22, 1.32, 1.39, 1.33, 1.54, 1.04, 2.25, 1.49)
D \leftarrow c(1.3, .75, 1.26, .69, .62, .9, 1.2, .32)
E <- c(.73, .8, .9, 1.24, .82, .72, .57, 1.18, .54, 1.3)
out2 <- makemultdata(A, B, C, D, E,
                      cuts = median(c(A, B, C, D, E)))
out2
## The reaction time data.
data(RTdata)
out3 <- makemultdata(RTdata, cuts =
                      100*c(5, 10, 12, 14, 16, 20, 25, 30, 40, 50))
dim(out3$y)
out3$y[1:10,]
```

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multmixEM	EM Algorithm for Mixtures of Multinomials	
multmixEM	EM Algorithm for Mixtures of Multinomials	

# Description

Return EM algorithm output for mixtures of multinomial distributions.

# Usage

```
multmixEM(y, lambda = NULL, theta = NULL, k = 2, maxit = 10000, epsilon = 1e-08, verb = FALSE)
```

# Arguments

•	,	
	У	Either An nxp matrix of data (multinomial counts), where n is the sample size and p is the number of multinomial bins, or the output of the makemultdata function. It is not necessary that all of the rows contain the same number of multinomial trials (i.e., the row sums of y need not be identical).
	lambda	Initial value of mixing proportions. Entries should sum to 1. This determines number of components. If NULL, then lambda is random from uniform Dirichlet and number of components is determined by theta.
	theta	Initial value of theta parameters. Should be a kxp matrix, where p is the number of columns of y and k is number of components. Each row of theta should sum to 1. If NULL, then each row is random from uniform Dirichlet. If both lambda and theta are NULL, then number of components is determined by k.
	k	Number of components. Ignored unless lambda and theta are NULL.
	epsilon	The convergence criterion.
	maxit	The maximum number of iterations.
	verb	If TRUE, then various updates are printed during each iteration of the algorithm.

# Value

multmixEM returns a list of class mixEM with items:

У	The raw data.
lambda	The final mixing proportions.
theta	The final multinomial parameters.
loglik	The final log-likelihood.
posterior	An nxk matrix of posterior probabilities for observations.
all.loglik	A vector of each iteration's log-likelihood.
restarts	The number of times the algorithm restarted due to unacceptable choice of initial values.
ft	A character vector giving the name of the function.

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### References

- McLachlan, G. J. and Peel, D. (2000) Finite Mixture Models, John Wiley & Sons, Inc.
- Elmore, R. T., Hettmansperger, T. P. and Xuan, F. (2004) The Sign Statistic, One-Way Layouts and Mixture Models, *Statistical Science* **19(4)**, 579–587.

#### See Also

```
compCDF, makemultdata, multmixmodel.sel
```

### **Examples**

multmixmodel.sel

Model Selection Mixtures of Multinomials

### **Description**

Assess the number of components in a mixture of multinomials model using the Akaike's information criterion (AIC), Schwartz's Bayesian information criterion (BIC), Bozdogan's consistent AIC (CAIC), and Integrated Completed Likelihood (ICL).

### Usage

```
multmixmodel.sel(y, comps = NULL, ...)
```

# **Arguments**

У	Either An nxp matrix of data (multinomial counts), where n is the sample size and p is the number of multinomial bins, or the output of the makemultdata function. It is not necessary that all of the rows contain the same number of multinomial trials (i.e., the row sums of y need not be identical).
comps	Vector containing the numbers of components to consider. If NULL, this is set to be 1:(max possible), where (max possible) is $floor((m+1)/2)$ and m is the minimum row sum of y.
	Additional arguments passed to multmixEM.

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# Value

multmixmodel.sel returns a table summarizing the AIC, BIC, CAIC, ICL, and log-likelihood values along with the winner (the number with the lowest aforementioned values).

### See Also

```
compCDF, makemultdata, multmixEM
```

### **Examples**

```
##Data generated using the multinomial cutpoint method. set.seed(100) x \leftarrow matrix(rpois(70, 6), 10, 7) x.new \leftarrow makemultdata(x, cuts = 5)
```

multmixmodel.sel(x.newy, comps = c(1,2), epsilon = 1e-03)

mvnormalmixEM

EM Algorithm for Mixtures of Multivariate Normals

# Description

Return EM algorithm output for mixtures of multivariate normal distributions.

# Usage

```
mvnormalmixEM(x, lambda = NULL, mu = NULL, sigma = NULL, k = 2, arbmean = TRUE, arbvar = TRUE, epsilon = 1e-08, maxit = 10000, verb = FALSE)
```

### **Arguments**

х	A matrix of size nxp consisting of the data.
lambda	Initial value of mixing proportions. Entries should sum to 1. This determines number of components. If NULL, then lambda is random from uniform Dirichlet and number of components is determined by mu.
mu	A list of size k consisting of initial values for the p-vector mean parameters. If NULL, then the vectors are generated from a normal distribution with mean and standard deviation according to a binning method done on the data. If both lambda and mu are NULL, then number of components is determined by sigma.
sigma	A list of size k consisting of initial values for the pxp variance-covariance matrices. If NULL, then sigma is generated using the data. If lambda, mu, and sigma are NULL, then number of components is determined by $k$ .
k	Number of components. Ignored unless lambda, mu, and sigma are all NULL.

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arbmean If TRUE, then the component densities are allowed to have different mus. If

FALSE, then a scale mixture will be fit.

arbvar If TRUE, then the component densities are allowed to have different sigmas. If

FALSE, then a location mixture will be fit.

epsilon The convergence criterion.

maxit The maximum number of iterations.

verb If TRUE, then various updates are printed during each iteration of the algorithm.

### Value

normalmixEM returns a list of class mixEM with items:

x The raw data.

lambda The final mixing proportions.

mu A list of with the final mean vectors.

sigma A list with the final variance-covariance matrices.

loglik The final log-likelihood.

posterior An nxk matrix of posterior probabilities for observations.

all.loglik A vector of each iteration's log-likelihood.

restarts The number of times the algorithm restarted due to unacceptable choice of initial

values.

ft A character vector giving the name of the function.

#### References

McLachlan, G. J. and Peel, D. (2000) Finite Mixture Models, John Wiley & Sons, Inc.

#### See Also

normalmixEM

### **Examples**

##Fitting randomly generated data with a 2-component location mixture of bivariate normals.

##Fitting randomly generated data with a 2-component scale mixture of bivariate normals.

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NOdata

Ethanol Fuel Data Set

# **Description**

This data set gives the equivalence ratios and peak nitrogen oxide emissions in a study using pure ethanol as a spark-ignition engine fuel.

### Usage

N0data

# **Format**

This data frame consists of:

- NOThe peak nitrogen oxide emission levels.
- EquivalenceThe equivalence ratios for the engine at compression ratios from 7.5 to 18.

### **Source**

Brinkman, N. D. (1981) Ethanol Fuel – A Single-Cylinder Engine Study of Efficiency and Exhaust Emissions, *S.A.E. Transactions*, 68.

### References

Hurn, M., Justel, A. and Robert, C. P. (2003) Estimating Mixtures of Regressions, *Journal of Computational and Graphical Statistics* **12**(1), 55–79.

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normalmixEM

EM Algorithm for Mixtures of Univariate Normals

### **Description**

Return EM algorithm output for mixtures of normal distributions.

### Usage

```
normalmixEM (x, lambda = NULL, mu = NULL, sigma = NULL, k = 2,
    mean.constr = NULL, sd.constr = NULL,
    epsilon = 1e-08, maxit = 1000, maxrestarts=20,
    verb = FALSE, fast=FALSE, ECM = FALSE,
    arbmean = TRUE, arbvar = TRUE)
```

### **Arguments**

x A vector of length n consisting of the data.

lambda Initial value of mixing proportions. Automatically repeated as necessary to pro-

duce a vector of length k, then normalized to sum to 1. If NULL, then lambda is random from a uniform Dirichlet distribution (i.e., its entries are uniform ran-

dom and then it is normalized to sum to 1).

mu Starting value of vector of component means. If non-NULL and a scalar, arbmean

is set to FALSE. If non-NULL and a vector, k is set to length(mu). If NULL, then the initial value is randomly generated from a normal distribution with cen-

ter(s) determined by binning the data.

sigma Starting value of vector of component standard deviations for algorithm. If non-

NULL and a scalar, arbvar is set to FALSE. If non-NULL and a vector, arbvar is set to TRUE and k is set to length(sigma). If NULL, then the initial value is the reciprocal of the square root of a vector of random exponential-distribution values whose means are determined according to a binning method done on the

data.

k Number of components. Initial value ignored unless mu and sigma are both

NULL.

mean.constr Equality constraints on the mean parameters, given as a vector of length k. Each

vector entry helps specify the constraints, if any, on the corresponding mean parameter: If NA, the corresponding parameter is unconstrained. If numeric, the corresponding parameter is fixed at that value. If a character string consisting of a single character preceded by a coefficient, such as "0.5a" or "-b", all parameters using the same single character in their constraints will fix these parameters equal to the coefficient times some the same free parameter. For instance, if mean.constr = c(NA, 0, "a", "-a"), then the first mean parameter is unconstrained, the second is fixed at zero, and the third and forth are constrained

to be equal and opposite in sign.

sd.constr Equality constraints on the standard deviation parameters. See mean.constr.

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epsilon The convergence criterion. Convergence is declared when the change in the

observed data log-likelihood increases by less than epsilon.

maxit The maximum number of iterations.

maxrestarts The maximum number of restarts allowed in case of a problem with the particu-

lar starting values chosen due to one of the variance estimates getting too small (each restart uses randomly chosen starting values). It is well-known that when each component of a normal mixture may have its own mean and variance, the likelihood has no maximizer; in such cases, we hope to find a "nice" local maximum with this algorithm instead, but occasionally the algorithm finds a "not nice" solution and one of the variances goes to zero, driving the likelihood to

infinity.

verb If TRUE, then various updates are printed during each iteration of the algorithm.

fast If TRUE and k==2 and arbmean==TRUE, then use normalmixEM2comp, which is a much faster version of the EM algorithm for this case. This version is less

is a much faster version of the EM algorithm for this case. This version is less protected against certain kinds of underflow that can cause numerical problems

and it does not permit any restarts. If k>2, fast is ignored.

ECM logical: Should this algorithm be an ECM algorithm in the sense of Meng and

Rubin (1993)? If FALSE, the algorithm is a true EM algorithm; if TRUE, then every half-iteration alternately updates the means conditional on the variances or the variances conditional on the means, with an extra E-step in between these

updates.

arbmean If TRUE, then the component densities are allowed to have different mus. If

FALSE, then a scale mixture will be fit. Initial value ignored unless mu is NULL.

arbvar If TRUE, then the component densities are allowed to have different sigmas. If

FALSE, then a location mixture will be fit. Initial value ignored unless sigma is

NULL.

### Details

This is the standard EM algorithm for normal mixtures that maximizes the conditional expected complete-data log-likelihood at each M-step of the algorithm. If desired, the EM algorithm may be replaced by an ECM algorithm (see ECM argument) that alternates between maximizing with respect to the mu and lambda while holding sigma fixed, and maximizing with respect to sigma and lambda while holding mu fixed. In the case where arbmean is FALSE and arbvar is TRUE, there is no closed-form EM algorithm, so the ECM option is forced in this case.

### Value

normalmixEM returns a list of class mixEM with items:

x The raw data.

1ambda The final mixing proportions.mu The final mean parameters.

sigma The final standard deviations. If arbmean = FALSE, then only the smallest stan-

dard deviation is returned. See scale below.

normalmixEM2comp

scale	If arbmean = FALSE, then the scale factor for the component standard deviations is returned. Otherwise, this is omitted from the output.
loglik	The final log-likelihood.
posterior	An nxk matrix of posterior probabilities for observations.
all.loglik	A vector of each iteration's log-likelihood. This vector includes both the initial and the final values; thus, the number of iterations is one less than its length.
restarts	The number of times the algorithm restarted due to unacceptable choice of initial values.
ft	A character vector giving the name of the function.

### References

- McLachlan, G. J. and Peel, D. (2000) Finite Mixture Models, John Wiley \& Sons, Inc.
- Meng, X.-L. and Rubin, D. B. (1993) Maximum Likelihood Estimation Via the ECM Algorithm: A General Framework, *Biometrika* 80(2): 267-278.
- Benaglia, T., Chauveau, D., Hunter, D. R., and Young, D. mixtools: An R package for analyzing finite mixture models. Journal of Statistical Software, 32(6):1-29, 2009.

### See Also

```
mvnormalmixEM, normalmixEM2comp, normalmixMMlc, spEMsymloc
```

### **Examples**

```
##Analyzing the Old Faithful geyser data with a 2-component mixture of normals.

data(faithful)
attach(faithful)
set.seed(100)
system.time(out<-normalmixEM(waiting, arbvar = FALSE, epsilon = 1e-03))
out
system.time(out2<-normalmixEM(waiting, arbvar = FALSE, epsilon = 1e-03, fast=TRUE))
out2 # same thing but much faster</pre>
```

normalmixEM2comp

Fast EM Algorithm for 2-Component Mixtures of Univariate Normals

# **Description**

Return EM algorithm output for mixtures of univariate normal distributions for the special case of 2 components, exploiting the simple structure of the problem to speed up the code.

### Usage

```
normalmixEM2comp(x, lambda, mu, sigsqrd, eps= 1e-8, maxit = 1000, verb=FALSE)
```

normalmixEM2comp 33

#### **Arguments**

 $\mathbf{x}$  A vector of length n consisting of the data.

lambda Initial value of first-component mixing proportion.

mu A 2-vector of initial values for the mean parameters.

sigsqrd Either a scalar or a 2-vector with initial value(s) for the variance parameters. If

a scalar, the algorithm assumes that the two components have equal variances; if a 2-vector, it assumes that the two components do not have equal variances.

eps The convergence criterion. Convergence is declared when the change in the

observed data log-likelihood increases by less than epsilon.

maxit The maximum possible number of iterations.

verb If TRUE, then various updates are printed during each iteration of the algorithm.

### **Details**

This code is written to be very fast, sometimes more than an order of magnitude faster than normalmixEM for the same problem. It is less numerically stable that normalmixEM in the sense that it does not safeguard against underflow as carefully.

Note that when the two components are assumed to have unequal variances, the loglikelihood is unbounded. However, in practice this is rarely a problem and quite often the algorithm converges to a "nice" local maximum.

#### Value

normalmixEM2comp returns a list of class mixEM with items:

x The raw data.

lambda The final mixing proportions (lambda and 1-lambda).

mu The final two mean parameters.

sigma The final one or two standard deviations.

loglik The final log-likelihood.

posterior An nx2 matrix of posterior probabilities for observations.

all.loglik A vector of each iteration's log-likelihood. This vector includes both the initial

and the final values; thus, the number of iterations is one less than its length.

restarts The number of times the algorithm restarted due to unacceptable choice of initial

values (always zero).

ft A character vector giving the name of the function.

#### References

McLachlan, G. J. and Peel, D. (2000) Finite Mixture Models, John Wiley & Sons, Inc.

#### See Also

mvnormalmixEM, normalmixEM

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### **Examples**

normalmixMMlc

EC-MM Algorithm for Mixtures of Univariate Normals with linear constraints

### Description

Return EC-MM (see below) algorithm output for mixtures of normal distributions with linear constraints on the means and variances parameters, as in Chauveau and Hunter (2013). The linear constraint for the means is of the form  $\mu=M\beta+C$ , where M and C are matrix and vector specified as parameters. The linear constraints for the variances are actually specified on the inverse variances, by  $\pi=A\gamma$ , where  $\pi$  is the vector of inverse variances, and A is a matrix specified as a parameter (see below).

### Usage

#### **Arguments**

x A vector of length n consisting of the data.

lambda Initial value of mixing proportions. Automatically repeated as necessary to pro-

duce a vector of length k, then normalized to sum to 1. If NULL, then lambda is random from a uniform Dirichlet distribution (i.e., its entries are uniform ran-

dom and then it is normalized to sum to 1).

Starting value of vector of component means. If non-NULL and a vector, k is

set to length(mu). If NULL, then the initial value is randomly generated from

a normal distribution with center(s) determined by binning the data.

mu

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sigma Starting value of vector of component standard deviations for algorithm. Obso-

lete for linear constraint on the inverse variances, use gparam instead to specify

a starting value. Note: This needs more precision

k Number of components. Initial value ignored unless mu and sigma are both

NULL.

mean.constr First, simplest way to define equality constraints on the mean parameters, given

as a vector of length k, like in normalmixEM. Each vector entry helps specify the constraints, if any, on the corresponding mean parameter: If NA, the corresponding parameter is unconstrained. If numeric, the corresponding parameter is fixed at that value. If a character string consisting of a single character preceded by a coefficient, such as "0.5a" or "-b", all parameters using the same single character in their constraints will fix these parameters equal to the coefficient times some the same free parameter. For instance, if mean.constr = c(NA, 0, "a", "-a"), then the first mean parameter is unconstrained, the second is fixed at zero, and the third and forth are constrained to be equal and opposite in sign. Note: if

there are no linear constraints for the variances, it is more efficient to use di-

rectly normalmixEM.

mean.lincstr Matrix M(k, p) in the linear constraint for the means equation  $\mu = M\beta + C$ ,

with  $p \leq k$ .

mean.constant Vector of k constants C in the linear constraint for the means equation  $\mu =$ 

 $M\beta + C$ .

var.lincstr Matrix A(k,q) in the linear constraint for the inverse variances equation  $\pi =$ 

 $A\gamma$ , with  $q \leq k$ .

gparam Vector of q starting values for the  $\gamma$  parameter in the linear constraint for the

inverse variances. This parameter is required.

epsilon The convergence criterion. Convergence is declared when the change in the

observed data log-likelihood increases by less than epsilon.

maxit The maximum allowed number of iterations.

maxrestarts The maximum number of restarts allowed in case of a problem with the particu-

lar starting values chosen due to one of the variance estimates getting too small (each restart uses randomly chosen starting values). It is well-known that when each component of a normal mixture may have its own mean and variance, the likelihood has no maximizer; in such cases, we hope to find a "nice" local maximum with this algorithm instead, but occasionally the algorithm finds a "not nice" solution and one of the variances goes to zero, driving the likelihood to

infinity.

verb If TRUE, then various updates are printed during each iteration of the algorithm.

### **Details**

This is a specific "EC-MM" algorithm for normal mixtures with linear constraints on the means and variances parameters. EC-MM here means that this algorithm is similar to an ECM algorithm as in Meng and Rubin (1993), except that it uses conditional MM (Minorization-Maximization)-steps instead of simple M-steps. Conditional means that it alternates between maximizing with respect to the mu and lambda while holding sigma fixed, and maximizing with respect to sigma and lambda while holding mu fixed. This ECM generalization of EM is forced in the case of linear constraints because there is no closed-form EM algorithm.

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### Value

normalmixMMlc returns a list of class mixEM with items:

x	The raw data.
lambda	The final mixing proportions.
mu	The final mean parameters.
sigma	The final standard deviations. If arbmean = FALSE, then only the smallest standard deviation is returned. See scale below.
scale	If arbmean = FALSE, then the scale factor for the component standard deviations is returned. Otherwise, this is omitted from the output.
loglik	The final log-likelihood.
posterior	An nxk matrix of posterior probabilities for observations.
all.loglik	A vector of each iteration's log-likelihood. This vector includes both the initial and the final values; thus, the number of iterations is one less than its length.
restarts	The number of times the algorithm restarted due to unacceptable choice of initial values.
beta	The final $\beta$ parameter estimate.
gamma	The final $\gamma$ parameter estimate.
ft	A character vector giving the name of the function.

# Author(s)

Didier Chauveau

### References

- McLachlan, G. J. and Peel, D. (2000) Finite Mixture Models, John Wiley & Sons, Inc.
- Meng, X.-L. and Rubin, D. B. (1993) Maximum Likelihood Estimation Via the ECM Algorithm: A General Framework, *Biometrika* 80(2): 267-278.
- Chauveau, D. and Hunter, D.R. (2013) ECM and MM algorithms for mixtures with constrained parameters, *preprint* http://hal.archives-ouvertes.fr/hal-00625285.
- Thomas, H., Lohaus, A., and Domsch, H. (2011), Extensions of Reliability Theory, in Non-parametric Statistics and Mixture Models: A Festschrift in Honor of Thomas Hettmansperger *Singapore: World Scientific*, pp. 309-316.

# See Also

normalmixEM, mvnormalmixEM, normalmixEM2comp

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## **Examples**

```
## Analyzing synthetic data as in the tau equivalent model
## From Thomas et al (2011), see also Chauveau and Hunter (2013)
## a 3-component mixture of normals with linear constraints.
1bd <- c(0.6,0.3,0.1); m <- length(1bd)
sigma \leftarrow sig0 \leftarrow sqrt(c(1,9,9))
# means constaints mu = M beta
M \leftarrow matrix(c(1,1,1,0,1,-1), 3, 2)
beta <- c(1,5) # unknown constained mean
mu0 <- mu <- as.vector(M %*% beta)
# linear constraint on the inverse variances pi = A.g
A <- matrix(c(1,1,1,0,1,0), m, 2, byrow=TRUE)
iv0 < -1/(sig0^2)
g0 <- c(iv0[2], iv0[1] - iv0[2]) # gamma^0 init
# simulation and EM fits
set.seed(40); n=100; x <- rnormmix(n,lbd,mu,sigma)
s <- normalmixEM(x,mu=mu0,sigma=sig0) # plain EM
# EM with var and mean linear constraints
sc <- normalmixMMlc(x, lambda=lbd, mu=mu0, sigma=sig0,</pre>
mean.lincstr=M, var.lincstr=A, gparam=g0)
# plot and compare both estimates
dnormmixt <- function(t, lam, mu, sig){</pre>
m <- length(lam); f <- 0</pre>
for (j in 1:m) f <- f + lam[j]*dnorm(t,mean=mu[j],sd=sig[j])</pre>
f}
t <- seq(min(x)-2, max(x)+2, len=200)
hist(x, freq=FALSE, col="lightgrey",
ylim=c(0,0.3), ylab="density",main="")
lines(t, dnormmixt(t, lbd, mu, sigma), col="darkgrey", lwd=2) # true
lines(t, dnormmixt(t, s$lambda, s$mu, s$sigma), lty=2)
lines(t, dnormmixt(t, sc$lambda, sc$mu, sc$sigma), col=1, lty=3)
legend("topleft", c("true", "plain EM", "constr EM"),
col=c("darkgrey",1,1), lty=c(1,2,3), lwd=c(2,1,1))
```

npEM

Nonparametric EM-like Algorithm for Mixtures of Independent Repeated Measurements

# **Description**

Returns nonparametric EM algorithm output (Benaglia et al, 2009) for mixtures of multivariate (repeated measures) data where the coordinates of a row (case) in the data matrix are assumed to be independent, conditional on the mixture component (subpopulation) from which they are drawn.

```
npEM(x, mu0, blockid = 1:ncol(x),
bw = bw.nrd0(as.vector(as.matrix(x))), samebw = TRUE,
```

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```
h = bw, eps = 1e-8,
maxiter = 500, stochastic = FALSE, verb = TRUE)
```

### **Arguments**

An  $n \times r$  matrix of data. Each of the n rows is a case, and each case has r

repeated measurements. These measurements are assumed to be conditionally independent, conditional on the mixture component (subpopulation) from which

the case is drawn.

mu0 Either an  $m \times r$  matrix specifying the initial centers for the kmeans function, or

an integer m specifying the number of initial centers, which are then choosen

randomly in kmeans

blockid A vector of length r identifying coordinates (columns of x) that are assumed

to be identically distributed (i.e., in the same block). For instance, the default has all distinct elements, indicating that no two coordinates are assumed identically distributed and thus a separate set of m density estimates is produced for each column of x. On the other hand, if blockid=rep(1,ncol(x)), then the

coordinates in each row are assumed conditionally i.i.d.

bw Bandwidth for density estimation, equal to the standard deviation of the kernel

density. By default, a simplistic application of the default bw.nrd0 bandwidth

used by density to the entire dataset.

samebw Logical: If TRUE, use the same bandwidth for each iteration and for each com-

ponent and block. If FALSE, use a separate bandwidth for each component and block, and update this bandwidth at each iteration of the algorithm using a suit-

ably modified bw.nrd0 method as described in Benaglia et al (2011).

h Alternative way to specify the bandwidth, to provide backward compatibility.

eps Tolerance limit for declaring algorithm convergence. Convergence is declared

whenever the maximum change in any coordinate of the lambda vector (of mix-

ing proportion estimates) does not exceed eps.

maxiter The maximum number of iterations allowed, for both stochastic and non-stochastic

versions; for non-stochastic algorithms (stochastic = FALSE), convergence

may be declared before maxiter iterations (see eps above).

stochastic Flag, if FALSE (the default), runs the non-stochastic version of the npEM algo-

rithm, as in Benaglia et al (2009). Set to TRUE to run a stochastic version which simulates the posteriors at each iteration, and runs for maxiter iterations.

verb If TRUE, print updates for every iteration of the algorithm as it runs

### Value

npEM returns a list of class npEM with the following items:

data The raw data (an  $n \times r$  matrix).

posteriors An  $n \times m$  matrix of posterior probabilities for observation. If stochastic = TRUE,

this matrix is computed from an average over the maxiter iterations.

bandwidth If samebw==TRUE, same as the bw input argument; otherwise, value of bw ma-

trix at final iteration. This information is needed by any method that produces

density estimates from the output.

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blockid Same as the blockid input argument, but recoded to have positive integer val-

ues. Also needed by any method that produces density estimates from the out-

put.

lambda The sequence of mixing proportions over iterations.

lambdahat The final mixing proportions if stochastic = FALSE, or the average mixing

proportions if stochastic = TRUE.

loglik The sequence of log-likelihoods over iterations.

#### References

• Benaglia, T., Chauveau, D., and Hunter, D. R. (2009), An EM-like algorithm for semi- and non-parametric estimation in multivariate mixtures, Journal of Computational and Graphical Statistics, 18, 505-526.

- Benaglia, T., Chauveau, D., Hunter, D. R., and Young, D. (2009), mixtools: An R package for analyzing finite mixture models. Journal of Statistical Software, 32(6):1-29.
- Benaglia, T., Chauveau, D. and Hunter, D.R. (2011), Bandwidth Selection in an EM-like algorithm for nonparametric multivariate mixtures. Nonparametric Statistics and Mixture Models:
   A Festschrift in Honor of Thomas P. Hettmansperger. World Scientific Publishing Co., pages 15-27.
- Bordes, L., Chauveau, D., and Vandekerkhove, P. (2007), An EM algorithm for a semiparametric mixture model, Computational Statistics and Data Analysis, 51: 5429-5443.

### See Also

```
plot.npEM, normmixrm.sim, spEMsymloc, spEM, plotseq.npEM
```

```
## Examine and plot water-level task data set.
## First, try a 3-component solution where no two coordinates are
## assumed i.d.
data(Waterdata)
set.seed(100)
## Not run:
a <- npEM(Waterdata[,3:10], mu0=3, bw=4) # Assume indep but not iid
plot(a) # This produces 8 plots, one for each coordinate
## End(Not run)
## Next, same thing but pairing clock angles that are directly opposite one
## another (1:00 with 7:00, 2:00 with 8:00, etc.)
## Not run:
b <- npEM(Waterdata[,3:10], mu0=3, blockid=c(4,3,2,1,3,4,1,2), bw=4) # iid in pairs
plot(b) # Now only 4 plots, one for each block
## End(Not run)</pre>
```

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npMSL

Nonparametric EM-like Algorithm for Mixtures of Independent Repeated Measurements - Maximum Smoothed Likelihood version

## **Description**

Returns nonparametric Smoothed Likelihood algorithm output (Levine et al, 2011) for mixtures of multivariate (repeated measures) data where the coordinates of a row (case) in the data matrix are assumed to be independent, conditional on the mixture component (subpopulation) from which they are drawn.

# Usage

```
npMSL(x, mu0, blockid = 1:ncol(x),
    bw = bw.nrd0(as.vector(as.matrix(x))), samebw = TRUE,
    bwmethod = "S", h = bw, eps = 1e-8,
    maxiter=500, bwiter = maxiter, nbfold = NULL,
    ngrid=200, post=NULL, verb = TRUE)
```

## **Arguments**

Х

An  $n \times r$  matrix of data. Each of the n rows is a case, and each case has r repeated measurements. These measurements are assumed to be conditionally independent, conditional on the mixture component (subpopulation) from which the case is drawn.

mu0

Either an  $m \times r$  matrix specifying the initial centers for the kmeans function, or an integer m specifying the number of initial centers, which are then choosen randomly in kmeans

blockid

A vector of length r identifying coordinates (columns of x) that are assumed to be identically distributed (i.e., in the same block). For instance, the default has all distinct elements, indicating that no two coordinates are assumed identically distributed and thus a separate set of m density estimates is produced for each column of x. On the other hand, if blockid=rep(1,ncol(x)), then the coordinates in each row are assumed conditionally i.i.d.

bw

Bandwidth for density estimation, equal to the standard deviation of the kernel density. By default, a simplistic application of the default bw.nrd0 bandwidth used by density to the entire dataset.

samebw

Logical: If TRUE, use the same bandwidth for each iteration and for each component and block. If FALSE, use a separate bandwidth for each component and block, and update this bandwidth at each iteration of the algorithm until bwiter is reached (see below). Two adaptation methods are provided, see bwmethod below.

bwmethod

Define the adaptive bandwidth strategy when samebw = FALSE, in which case the bandwidth depends on each component, block, and iteration of the algorithm. If set to "S" (the default), adaptation is done using a suitably modified

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bw.nrd0 method as described in Benaglia et al (2011). If set to "CV", an adaptive k-fold Cross Validation method is applied, as described in Chauveau et al (2014), where nbfold is the number of subsamples. This corresponds to a Leave-[n/nbfold]-Out CV.

h Alternative way to specify the bandwidth, to provide backward compatibility.

eps Tolerance limit for declaring algorithm convergence. Convergence is declared

whenever the maximum change in any coordinate of the lambda vector (of mix-

ing proportion estimates) does not exceed eps.

maxiter The maximum number of iterations allowed, convergence may be declared be-

fore maxiter iterations (see eps above).

bwiter The maximum number of iterations allowed for adaptive bandwidth stage, when

samebw = FALSE. If set to 0, then the initial bandwidth matrix is used without

adaptation.

nbfold A parameter passed to the internal function wbs. kCV, which controls the weighted

bandwidth selection by k-fold cross-validation.

ngrid Number of points in the discretization of the intervals over which are approxi-

mated the (univariate) integrals for non linear smoothing of the log-densities, as

required in the E step of the npMSL algorithm, see Levine et al (2011).

post If non-NULL, an  $n \times m$  matrix specifying the initial posterior probability vectors

for each of the observations, i.e., the initial values to start the EM-like algorithm.

verb If TRUE, print updates for every iteration of the algorithm as it runs

### Value

npMSL returns a list of class npEM with the following items:

data The raw data (an  $n \times r$  matrix).

posteriors An  $n \times m$  matrix of posterior probabilities for observation.

bandwidth If samebw==TRUE, same as the bw input argument; otherwise, value of bw ma-

trix at final iteration. This information is needed by any method that produces

density estimates from the output.

blockid Same as the blockid input argument, but recoded to have positive integer val-

ues. Also needed by any method that produces density estimates from the out-

put.

lambda The sequence of mixing proportions over iterations.

lambdahat The final mixing proportions.

loglik The sequence of log-likelihoods over iterations.

f An array of size  $nqrid \times m \times l$ , returning last values of density for component

j and block k over grid points.

meanNaN Average number of NaN that occured over iterations (for internal testing and

control purpose).

meanUdf1 Average number of "underflow" that occured over iterations (for internal testing

and control purpose).

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## References

• Benaglia, T., Chauveau, D., and Hunter, D. R. (2009), An EM-like algorithm for semi- and non-parametric estimation in multivariate mixtures, Journal of Computational and Graphical Statistics, 18, 505-526.

- Benaglia, T., Chauveau, D. and Hunter, D.R. (2011), Bandwidth Selection in an EM-like algorithm for nonparametric multivariate mixtures. Nonparametric Statistics and Mixture Models: A Festschrift in Honor of Thomas P. Hettmansperger. World Scientific Publishing Co., pages 15-27.
- Chauveau D., Hunter D. R. and Levine M. (2014), Semi-Parametric Estimation for Conditional Independence Multivariate Finite Mixture Models. Preprint (under revision).
- Levine, M., Hunter, D. and Chauveau, D. (2011), Maximum Smoothed Likelihood for Multivariate Mixtures, Biometrika 98(2): 403-416.

### See Also

```
npEM, plot.npEM, normmixrm.sim, spEMsymloc, spEM, plotseq.npEM
```

```
## Examine and plot water-level task data set.
## Block structure pairing clock angles that are directly opposite one
## another (1:00 with 7:00, 2:00 with 8:00, etc.)
set.seed(111) # Ensure that results are exactly reproducible
data(Waterdata)
blockid \leftarrow c(4,3,2,1,3,4,1,2) # see Benaglia et al (2009a)
## Not run:
a <- npEM(Waterdata[,3:10], mu0=3, blockid=blockid, bw=4) # npEM solution
b <- npMSL(Waterdata[,3:10], mu0=3, blockid=blockid, bw=4) # smoothed version
# Comparisons on the 4 default plots, one for each block
par(mfrow=c(2,2))
for (l in 1:4){
plot(a, blocks=1, breaks=5*(0:37)-92.5,
xlim=c(-90,90), xaxt="n",ylim=c(0,.035), xlab="")
plot(b, blocks=1, hist=FALSE, newplot=FALSE, addlegend=FALSE, lty=2,
dens.col=1)
axis(1, at=30*(1:7)-120, cex.axis=1)
legend("topleft",c("npMSL"),lty=2, lwd=2)}
## End(Not run)
```

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# **Description**

Takes an object of class mixEM and returns various graphical output for select mixture models.

### Usage

```
## S3 method for class 'mixEM'
plot(x, whichplots = 1,
loglik = 1 %in% whichplots,
density = 2 %in% whichplots,
xlab1="Iteration", ylab1="Log-Likelihood",
main1="Observed Data Log-Likelihood", col1=1, lwd1=2,
xlab2=NULL, ylab2=NULL, main2=NULL, col2=NULL,
lwd2=2,
alpha = 0.05, marginal = FALSE, ...)
```

## **Arguments**

x	An object of class mixEM.
whichplots	vector telling which plots to produce: $1 = loglikelihood plot$ , $2 = density plot$ . Irrelevant if $loglik$ and density are specified.
loglik	If TRUE, a plot of the log-likelihood versus the EM iterations is given.
density	Graphics pertaining to certain mixture models. The details are given below.
xlab1, ylab1, m	nain1, col1, lwd1
	Graphical parameters xlab,, lwd to be passed to the loglikelihood plot. Trying to change these parameters using xlab,, lwd will result in an error, but all other graphical parameters are passed directly to the plotting functions via
xlab2, ylab2, m	main2, col2, lwd2
	Same as xlab1 etc. but for the density plot
alpha	A vector of significance levels when constructing confidence ellipses and confidence bands for the mixture of multivariate normals and mixture of regressions cases, respectively. The default is 0.05.
marginal	For the mixture of bivariate normals, should optional marginal histograms be included?

## Value

. . .

plot.mixEM returns a plot of the log-likelihood versus the EM iterations by default for all objects of class mixEM. In addition, other plots may be produced for the following k-component mixture model functions:

Graphical parameters passed to plot command.

normalmixEM A histogram of the raw data is produced along with k density curves determined by normalmixEM.

A histogram of the raw data produced in a similar manner as for normalmixEM.

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mvnormalmixEM

A 2-dimensional plot with each point color-coded to denote its most probable component membership. In addition, the estimated component means are plotted along with (1 - alpha)% bivariate normal density contours. These ellipses are constructed by assigning each value to their component of most probable membership and then using normal theory. Optional marginal histograms may also be produced.

regmixEM

A plot of the response versus the predictor with each point color-coded to denote its most probable component membership. In addition, the estimated component regression lines are plotted along with (1 - alpha)% Working-Hotelling confidence bands. These bands are constructed by assigning each value to their component of most probable membership and then performing least squares estimation.

logisregmixEM

A plot of the binary response versus the predictor with each point color-coded to denote its most probable compopnent membership. In addition, the estimate component logistic regression lines are plotted.

regmixEM.mixed Provides a 2x2 matrix of plots summarizing the posterior slope and posterior intercept terms from a mixture of random effects regression. See post.beta for a more detailed description.

## See Also

post.beta

```
##Analyzing the Old Faithful geyser data with a 2-component mixture of normals.
data(faithful)
attach(faithful)
set.seed(100)
out <- normalmixEM(waiting, arbvar = FALSE, verb = TRUE,
                   epsilon = 1e-04)
plot(out, density = TRUE, w = 1.1)
##Fitting randomly generated data with a 2-component location mixture of bivariate normals.
x.1 < - rmvnorm(40, c(0, 0))
x.2 < - rmvnorm(60, c(3, 4))
X.1 <- rbind(x.1, x.2)
out.1 <- mvnormalmixEM(X.1, arbvar = FALSE, verb = TRUE,
                       epsilon = 1e-03)
plot(out.1, density = TRUE, alpha = c(0.01, 0.05, 0.10),
     marginal = TRUE)
```

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plot.mixMCMC Variou Metho	Plots Pertaining to Mixture Model Output Using MCMC
---------------------------	---

# Description

Takes an object of class mixMCMC and returns various graphical output for select mixture models.

# Usage

```
## S3 method for class 'mixMCMC'
plot(x, trace.plots = TRUE,
    summary.plots = FALSE, burnin = 2000, ...)
```

## **Arguments**

An object of class mixMCMC.

trace.plots

If TRUE, trace plots of the various parameters estimated by the MCMC methods is given.

summary.plots

Graphics pertaining to certain mixture models. The details are given below.

The values 1 to burnin are dropped when producing the plots in summary.plots.

Graphical parameters passed to regcr function.

### Value

plot.mixMCMC returns trace plots of the various parameters estimated by the MCMC methods for all objects of class mixMCMC. In addition, other plots may be produced for the following k-component mixture model functions:

regmixMH Credible bands for the regression lines in a mixture of linear regressions. See regcr for more details.

## See Also

regcr

```
## M-H algorithm for NOdata with acceptance rate about 40%.

data(NOdata)
attach(NOdata)
set.seed(100)
beta <- matrix(c(1.3, -0.1, 0.6, 0.1), 2, 2)
sigma <- c(.02, .05)
MH.out <- regmixMH(Equivalence, NO, beta = beta, s = sigma,</pre>
```

plot.npEM

```
sampsize = 2500, omega = .0013)
plot(MH.out, summary.plots = TRUE, burnin = 2450,
    alpha = 0.01)
```

plot.npEM

Plot Nonparametric or Semiparametric EM Output

## **Description**

Takes an object of class npEM and returns a set of plots of the density estimates for each block and each component. There is one plot per block, with all the components displayed on each block so it is possible to see the mixture structure for each block.

# Usage

## **Arguments**

X	An object of class npEM such as the output of the npEM function
blocks	Blocks (of repeated measures coordinates) to plot; not relevant for univariate case. Default is to plot all blocks.
hist	If TRUE, superimpose density estimate plots on a histogram of the data
addlegend	If TRUE, adds legend to the plot.
scale	If TRUE, scale each density estimate by its corresponding estimated mixing proportion, so that the total area under all densities equals 1 and the densities plotted may be added to produce an estimate of the mixture density. When FALSE, each density curve has area 1 in the plot.
title	Alternative vector of main titles for plots (recycled as many times as needed)
breaks	Passed directly to the hist function
ylim	ylim parameter to use for all plots, if desired. If not given, each plot uses its own ylim that ensures that no part of the plot will go past the top of the plotting area.
dens.col	Color values to use for the individual component density functions, repeated as necessary. Default value is 2: (m+1).
newplot	If TRUE, creates a new plot.
pos.legend	Single argument specifying the position of the legend. See 'Details' section of legend.

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```
cex.legend Character expansion factor for legend.... Any remaining arguments are passed to the hist and lines functions.
```

#### Value

plot.npEM returns a list with two elements:

x List of matrices. The jth column of the ith matrix is the vector of x-values for the jth density in the ith plot.

y y-values, given in the same form as the x-values.

### See Also

```
npEM, density.npEM, spEMsymloc, plotseq.npEM
```

# **Examples**

```
## Examine and plot water-level task data set.
## First, try a 3-component solution where no two coordinates are
## assumed i.d.
data(Waterdata)
set.seed(100)
## Not run:
a <- npEM(Waterdata[,3:10], 3, bw=4)</pre>
par(mfrow=c(2,4))
plot(a) # This produces 8 plots, one for each coordinate
## End(Not run)
## Not run:
## Next, same thing but pairing clock angles that are directly opposite one
## another (1:00 with 7:00, 2:00 with 8:00, etc.)
b <- npEM(Waterdata[,3:10], 3, blockid=c(4,3,2,1,3,4,1,2), bw=4)
par(mfrow=c(2,2))
plot(b) # Now only 4 plots, one for each block
## End(Not run)
```

plot.spEMN01

Plot mixture pdf for the semiparametric mixture model output by spEMsymlocN01

# **Description**

Plot mixture density for the semiparametric mixture model output by spEMsymlocN01, with one component known and set to normal(0,1), and a symmetric nonparametric density with location parameter.

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## Usage

```
## S3 method for class 'spEMN01'
plot(x, bw = x$bandwidth, knownpdf = dnorm, add.plot = FALSE, ...)
```

## **Arguments**

x An object of class "spEMN01" as returned by spEMsymlocN01

bw Bandwidth for weighted kernel density estimation.

knownpdf The known density of component 1, default to dnorm.

add.plot Set to TRUE to add to an existing plot.

... further arguments passed to plot if add.plot = FALSE, and to lines if add.plot = TRUE.

### Value

A plot of the density of the mixture

### Author(s)

Didier Chauveau

## References

 Chauveau, D., Saby, N., Orton, T. G., Lemercier B., Walter, C. and Arrouys, D. Large-scale simultaneous hypothesis testing in soil monitoring: A semi-parametric mixture approach, preprint (2013).

### See Also

spEMsymlocN01

plotFDR	Plot False Discovery Rate (FDR) estimates from output by EM-like
	strategies

## **Description**

Plot  $FDR(p_i)$  estimates against index of sorted p-values from, e.g., normalmixEM or the semiparametric mixture model posterior probabilities output by pEMsymlocN01, or any EM-algorithm like pormalmixEM which returns posterior probabilities. The function can simultaneously plot FDR estimates from two strategies for comparison. Plot of the true FDR can be added if complete data are available (typically in simulation studies).

```
plotFDR (post1, post2 = NULL, lg1 = "FDR 1", lg2 = NULL, title = NULL, compH0 = 1, alpha = 0.1, complete.data = NULL, pctfdr = 0.3)
```

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# **Arguments**

post1	The posterior probabilities from objects such as the output from spEMsymlocN01.
post2	A second object like post1 if comparison is desired.
lg1	Text describing the FDR estimate in post1.
lg2	Text describing the FDR estimate in post2 if provided.
title	Plot title, a default is provided if NULL.
compH0	The component indicator associated to the null hypothesis H0, normally 1 since it is defined in this way in spEMsymlocN01, but in case of label switching in other algorithms it can be set to 2.
alpha	The target FDR level; the index at which the FDR estimate crosses the horizontal line for level alpha gives the maximum number of cases to reject.
complete.data	An array with $n$ lines and 2 columns, with the component indicator in column 1 and the p-values in column 2, sorted by p-values.
pctfdr	The level up to which the FDR is plotted, i.e. the scale of the vertical axis.

# Value

A plot of one or two FDR estimates, with the true FDR if available

# Author(s)

Didier Chauveau

# References

Chauveau, D., Saby, N., Orton, T. G., Lemercier B., Walter, C. and Arrouys, D. Large-scale simultaneous hypothesis testing in monitoring carbon content from French soil database – A semi-parametric mixture approach, Geoderma 219-220 (2014), 117-124.

# See Also

spEMsymlocN01

plotseq.npEM	Plotting sequences of estimates from non- or semiparametric EM-like Algorithm

# Description

Returns plots of the sequences of scalar parameter estimates along iterations from an object of class npEM.

```
## S3 method for class 'npEM' plotseq(x, ...)
```

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# Arguments

```
x an object of class npEM, as output by npEM or spEMsymloc
... further parameters that are passed to plot
```

#### **Details**

plotseq.npEM returns a figure with one plot for each component proportion, and, in the case of spEMsymloc, one plot for each component mean.

### References

- Benaglia, T., Chauveau, D., and Hunter, D. R. (2009), An EM-like algorithm for semi- and non-parametric estimation in multivariate mixtures, Journal of Computational and Graphical Statistics (to appear).
- Bordes, L., Chauveau, D., and Vandekerkhove, P. (2007), An EM algorithm for a semiparametric mixture model, Computational Statistics and Data Analysis, 51: 5429-5443.

### See Also

```
plot.npEM, rnormmix, npEM, spEMsymloc
```

# **Examples**

```
## Example from a normal location mixture
n <- 200
set.seed(100)
lambda <- c(1/3,2/3)
mu <- c(0, 4); sigma<-rep(1, 2)
x <- rnormmix(n, lambda, mu, sigma)
b <- spEMsymloc(x, mu0=c(-1, 2), stochastic=FALSE)
plotseq(b)
bst <- spEMsymloc(x, mu0=c(-1, 2), stochastic=TRUE)
plotseq(bst)</pre>
```

poisregmixEM

EM Algorithm for Mixtures of Poisson Regressions

### **Description**

Returns EM algorithm output for mixtures of Poisson regressions with arbitrarily many components.

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# **Arguments**

y An n-vector of response values.

x An nxp matrix of predictors. See addintercept below.

lambda Initial value of mixing proportions. Entries should sum to 1. This determines

number of components. If NULL, then lambda is random from uniform Dirich-

let and number of components is determined by beta.

beta Initial value of beta parameters. Should be a pxk matrix, where p is the num-

ber of columns of x and k is number of components. If NULL, then beta is generated by binning the data into k bins and using glm on the values in each of the bins. If both lambda and beta are NULL, then number of components is

determined by k.

k Number of components. Ignored unless lambda and beta are both NULL.

addintercept If TRUE, a column of ones is appended to the x matrix before the value of p is

calculated.

epsilon The convergence criterion.

maxit The maximum number of iterations.

verb If TRUE, then various updates are printed during each iteration of the algorithm.

### Value

poisregmixEM returns a list of class mixEM with items:

x The predictor values.

y The response values.

lambda The final mixing proportions.

beta The final Poisson regression coefficients.

loglik The final log-likelihood.

posterior An nxk matrix of posterior probabilities for observations.

all.loglik A vector of each iteration's log-likelihood.

restarts The number of times the algorithm restarted due to unacceptable choice of initial

values

ft A character vector giving the name of the function.

### References

McLachlan, G. J. and Peel, D. (2000) Finite Mixture Models, John Wiley & Sons, Inc.

Wang, P., Puterman, M. L., Cockburn, I. and Le, N. (1996) Mixed Poisson Regression Models with Covariate Dependent Rates, *Biometrics*, **52(2)**, 381–400.

### See Also

logisregmixEM

52 print.npEM

## **Examples**

```
## EM output for data generated from a 2-component model.

set.seed(100)
beta <- matrix(c(1, .5, .7, -.8), 2, 2)
x <- runif(50, 0, 10)
xbeta <- cbind(1, x)%*%beta
w <- rbinom(50, 1, .5)
y <- w*rpois(50, exp(xbeta[, 1]))+(1-w)*rpois(50, exp(xbeta[, 2]))
out <- poisregmixEM(y, x, verb = TRUE, epsilon = 1e-03)
out</pre>
```

print.npEM

Printing non- and semi-parametric multivariate mixture model fits

# **Description**

print method for class npEM.

## Usage

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

# **Arguments**

x an object of class npEM such as a result of a call to npEM

... Additional arguments to print

## **Details**

print.npEM prints the elements of an npEM object without printing the data or the posterior probabilities. (These may still be accessed as x\$data and x\$posteriors.)

# Value

print.npEM returns (invisibly) the full value of x itself, including the data and posteriors elements.

## See Also

```
npEM, plot.npEM summary.npEM
```

```
data(Waterdata)
set.seed(100)
## Not run: npEM(Waterdata[,3:10], 3, bw=4, verb=FALSE) # Assume indep but not iid
```

RanEffdata 53

RanEffdata	Simulated Data from 2-Component Mixture of Regressions with Random Effects

# **Description**

This data set was generated from a 2-component mixture of regressions with random effects.

# Usage

RanEffdata

# **Format**

This data set consists of a list with 100 25x3 matrices. The first column is the response variable, the second column is a column of 1's and the last column is the predictor variable.

## See Also

regmixEM.mixed

regcr	Add a Confidence Region or Bayesian Credible Region for Regression
	Lines to a Scatterplot

# **Description**

Produce a confidence or credible region for regression lines based on a sample of bootstrap beta values or posterior beta values. The beta parameters are the intercept and slope from a simple linear regression.

# Usage

# Arguments

beta	An nx2 matrix of regression parameters. The first column gives the intercepts and the second column gives the slopes.
X	An n-vector of the predictor variable which is necessary when nonparametric = TRUE.
em.beta	The estimates for beta required when obtaining confidence regions. This is required for performing the standardization necessary when obtaining nonparametric confidence regions.

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em.sigma The estimates for the regression standard deviation required when obtaining

confidence regions. This is required for performing the standardization nec-

essary when obtaining nonparametric confidence regions.

alpha The proportion of the beta sample to remove. In other words, 1-alpha is the level

of the credible region.

nonparametric If nonparametric = TRUE, then the region is based on the convex hull of the

remaining beta after trimming, which is accomplished using a data depth technique. If nonparametric = FALSE, then the region is based on the asymptotic

normal approximation.

plot If plot = TRUE, lines are added to the existing plot. The type of plot created

depends on the value of xyaxes.

xyaxes If xyaxes = TRUE and plot = TRUE, then a confidence or credible region for the

regression lines is plotted on the x-y axes, presumably overlaid on a scatterplot of the data. If xyaxes = FALSE and plot = TRUE, the (convex) credible region for the regression line is plotted on the beta, or intercept-slope, axes, presumably

overlaid on a scatterplot of beta.

... Graphical parameters passed to lines or plot command.

### Value

reger returns a list containing the following items:

boundary A matrix of points in beta, or intercept-slope, space arrayed along the boundary

of the confidence or credible region.

upper A matrix of points in x-y space arrayed along the upper confidence or credible

limit for the regression line.

lower A matrix of points in x-y space arrayed along the lower confidence or credible

limit for the regression line.

### See Also

```
regmixEM, regmixMH
```

regmixEM 55

```
col = 2)
regcr(beta.c2, x = NO, nonparametric = TRUE, plot = TRUE,
      col = 3)
```

regmixEM

EM Algorithm for Mixtures of Regressions

# Description

Returns EM algorithm output for mixtures of multiple regressions with arbitrarily many components.

# Usage

# **Arguments**

 Samones	
У	An n-vector of response values.
X	An nxp matrix of predictors. See addintercept below.
lambda	Initial value of mixing proportions. Entries should sum to 1. This determines number of components. If NULL, then lambda is random from uniform Dirichlet and number of components is determined by beta.
beta	Initial value of beta parameters. Should be a pxk matrix, where p is the number of columns of x and k is number of components. If NULL, then beta has standard normal entries according to a binning method done on the data. If both lambda and beta are NULL, then number of components is determined by sigma.
sigma	A vector of standard deviations. If NULL, then 1/sigma^2 has random standard exponential entries according to a binning method done on the data. If lambda, beta, and sigma are NULL, then number of components is determined by k.
k	Number of components. Ignored unless all of lambda, beta, and sigma are NULL. $ \\$
addintercept	If TRUE, a column of ones is appended to the x matrix before the value of p is calculated.
arbmean	If TRUE, each mixture component is assumed to have a different set of regression coefficients (i.e., the betas).
arbvar	If TRUE, each mixture component is assumed to have a different sigma.
epsilon	The convergence criterion.
maxit	The maximum number of iterations.
verb	If TRUE, then various updates are printed during each iteration of the algorithm.

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## Value

regmixEM returns a list of class mixEM with items:

x The set of predictors (which includes a column of 1's if addintercept = TRUE).

y The response values.

lambda The final mixing proportions.

beta The final regression coefficients.

sigma The final standard deviations. If arbmean = FALSE, then only the smallest stan-

dard deviation is returned. See scale below.

scale If arbmean = FALSE, then the scale factor for the component standard devia-

tions is returned. Otherwise, this is omitted from the output.

loglik The final log-likelihood.

posterior An nxk matrix of posterior probabilities for observations.

all.loglik A vector of each iteration's log-likelihood.

restarts The number of times the algorithm restarted due to unacceptable choice of initial

values.

ft A character vector giving the name of the function.

### References

de Veaux, R. D. (1989), Mixtures of Linear Regressions, *Computational Statistics and Data Analysis* 8, 227-245.

Hurn, M., Justel, A. and Robert, C. P. (2003) Estimating Mixtures of Regressions, *Journal of Computational and Graphical Statistics* **12**(1), 55–79.

McLachlan, G. J. and Peel, D. (2000) Finite Mixture Models, John Wiley & Sons, Inc.

## See Also

```
regcr, regmixMH
```

```
## EM output for NOdata.

data(NOdata)
attach(NOdata)
set.seed(100)
em.out <- regmixEM(Equivalence, NO, verb = TRUE, epsilon = 1e-04)
em.out[3:6]</pre>
```

regmixEM.lambda 57

regmixEM.lambda <i>EM.</i>	Algorithm for Mixtures of Regressions with Local Lambda Estites
----------------------------	---

# Description

Returns output for one step of an EM algorithm output for mixtures of multiple regressions where the mixing proportions are estimated locally.

# Usage

```
regmixEM.lambda(y, x, lambda = NULL, beta = NULL, sigma = NULL,
                k = 2, addintercept = TRUE, arbmean = TRUE,
                arbvar = TRUE, epsilon = 1e-8, maxit = 10000,
                verb = FALSE)
```

# Arg

ŗ	guments		
	у	An n-vector of response values.	
	X	An nxp matrix of predictors. See addintercept below.	
	lambda	An nxk matrix of initial local values of mixing proportions. Entries should sum to 1. This determines number of components. If NULL, then lambda is simply one over the number of components.	
	beta	Initial value of beta parameters. Should be a pxk matrix, where p is the number of columns of x and k is number of components. If NULL, then beta has uniform standard normal entries. If both lambda and beta are NULL, then number of components is determined by sigma.	
	sigma	k-vector of initial global values of standard deviations. If NULL, then $1/\text{sigma}^2$ has random standard exponential entries. If lambda, beta, and sigma are NULL, then number of components is determined by k.	
	k	The number of components. Ignored unless all of lambda, beta, and sigma are NULL. $ \label{eq:number}$	
	addintercept	If TRUE, a column of ones is appended to the x matrix before the value of p is calculated.	
	arbmean	If TRUE, each mixture component is assumed to have a different set of regression coefficients (i.e., the betas).	
	arbvar	If TRUE, each mixture component is assumed to have a different sigma.	
	epsilon	The convergence criterion.	
	maxit	The maximum number of iterations.	
	verb	If TRUE, then various updates are printed during each iteration of the algorithm.	

# **Details**

Primarily used within regmixEM.loc.

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## Value

regmixEM.lambda returns a list of class mixEM with items:

x The set of predictors (which includes a column of 1's if addintercept = TRUE).

y The response values.

1ambda The inputted mixing proportions.beta The final regression coefficients.

sigma The final standard deviations. If arbmean = FALSE, then only the smallest stan-

dard deviation is returned. See scale below.

scale If arbmean = FALSE, then the scale factor for the component standard devia-

tions is returned. Otherwise, this is omitted from the output.

loglik The final log-likelihood.

posterior An nxk matrix of posterior probabilities for observations.

all.loglik A vector of each iteration's log-likelihood.

restarts The number of times the algorithm restarted due to unacceptable choice of initial

values.

ft A character vector giving the name of the function.

# See Also

```
regmixEM.loc
```

## **Examples**

```
## Compare a 2-component and 3-component fit to NOdata.

data(NOdata)
attach(NOdata)
set.seed(100)
out1 <- regmixEM.lambda(Equivalence, NO)
out2 <- regmixEM.lambda(Equivalence, NO, k = 3)
c(out1$loglik, out2$loglik)</pre>
```

regmixEM.loc Iterative Algorithm Using EM Algorithm for Mixtures of Regressions with Local Lambda Estimates

## **Description**

Iterative algorithm returning EM algorithm output for mixtures of multiple regressions where the mixing proportions are estimated locally.

regmixEM.loc 59

## Usage

## **Arguments**

У	An n-vector of response values.

x An nxp matrix of predictors. See addintercept below.

lambda An nxk matrix of initial local values of mixing proportions. Entries should sum

to 1. This determines number of components. If NULL, then lambda is simply

one over the number of components.

beta Initial global values of beta parameters. Should be a pxk matrix, where p is the

number of columns of x and k is number of components. If NULL, then beta has uniform standard normal entries. If both lambda and beta are NULL, then

number of components is determined by sigma.

sigma A k-vector of initial global values of standard deviations. If NULL, then 1/sigma<sup>2</sup>

has random standard exponential entries. If lambda, beta, and sigma are NULL,

then number of components determined by k.

k Number of components. Ignored unless all of lambda, beta, and sigma are

NULL.

addintercept If TRUE, a column of ones is appended to the x matrix before the value of p is

calculated.

kern.l The type of kernel to use in the local estimation of lambda.

epsilon The convergence criterion.

maxit The maximum number of iterations.

kernl.g A shape parameter required for the symmetric beta kernel for local estimation

of lambda. The default is g = 0 which yields the uniform kernel. Some common values are g = 1 for the Epanechnikov kernel, g = 2 for the biweight kernel, and

g = 3 for the triweight kernel.

kernl.h The bandwidth controlling the size of the window used in the local estimation

of lambda around x.

verb If TRUE, then various updates are printed during each iteration of the algorithm.

# Value

regmixEM. loc returns a list of class mixEM with items:

x The set of predictors (which includes a column of 1's if addintercept = TRUE).

y The response values.

lambda.x The final local mixing proportions.

beta The final global regression coefficients.

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sigma The final global standard deviations.

loglik The final log-likelihood.

posterior An nxk matrix of posterior probabilities for observations.

all.loglik A vector of each iteration's log-likelihood.

restarts The number of times the algorithm restarted due to unacceptable choice of initial values.

ft A character vector giving the name of the function.

## See Also

```
regmixEM.lambda
```

## **Examples**

regmixEM.mixed

EM Algorithm for Mixtures of Regressions with Random Effects

# **Description**

Returns EM algorithm output for mixtures of multiple regressions with random effects and an option to incorporate fixed effects and/or AR(1) errors.

regmixEM.mixed 61

Arg	um	ents

A list of N response trajectories with (possibly) varying dimensions of length У A list of N design matrices of dimensions  $(n_i) \times p$ . Each trajectory in y has its Х own design matrix. A list of N known explanatory variables having dimensions  $(n_i) \times q$ . If mixed = FALSE, then w is replaced by a list of N zeros. A vector of standard deviations. If NULL, then  $1/s^2$  has random standard exsigma ponential entries according to a binning method done on the data. arb.sigma If TRUE, then sigma is k-dimensional. Else a common standard deviation is assumed. alpha A q-vector of unknown regression parameters for the fixed effects. If NULL and mixed = TRUE, then alpha is random from a normal distribution with mean and variance according to a binning method done on the data. If mixed = FALSE, then alpha = 0. lambda Initial value of mixing proportions for the assumed mixture structure on the regression coefficients. Entries should sum to 1. This determines number of components. If NULL, then lambda is random from uniform Dirichlet and the number of components is determined by mu. A pxk matrix of the mean for the mixture components of the random regression mu coefficients. If NULL, then the columns of mu are random from a multivariate normal distribution with mean and variance determined by a binning method done on the data. rho An Nxk matrix giving initial values for the correlation term in an AR(1) process. If NULL, then these values are simulated from a uniform distribution on the interval (-1, 1). R A list of N pxp covariance matrices for the mixture components of the random regression coefficients. If NULL, then each matrix is random from a standard Wishart distribution according to a binning method done on the data. arb.R If TRUE, then R is a list of N pxp covariance matrices. Else, one common covariance matrix is assumed. k Number of components. Ignored unless lambda is NULL. If TRUE, then an AR(1) process on the error terms is included. The default is ar.1 FALSE. addintercept.fixed If TRUE, a column of ones is appended to the matrices in w. addintercept.random If TRUE, a column of ones is appended to the matrices in x before p is calcuepsilon The convergence criterion. The maximum number of iterations. maxit verb If TRUE, then various updates are printed during each iteration of the algorithm.

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### Value

regmixEM returns a list of class mixEM with items:

x The predictor values corresponding to the random effects.

y The response values.

The predictor values corresponding to the (optional) fixed effects.

lambda The final mixing proportions.

mu The final mean vectors.

R The final covariance matrices.

sigma The final component error standard deviations.

alpha The final regression coefficients for the fixed effects.

rho The final error correlation values if an AR(1) process is included.

loglik The final log-likelihood.

posterior.z An Nxk matrix of posterior membership probabilities.

posterior.beta A list of N pxk matrices giving the posterior regression coefficient values.

all.loglik A vector of each iteration's log-likelihood.

restarts The number of times the algorithm restarted due to unacceptable choice of initial

values.

ft A character vector giving the name of the function.

## References

Xu, W. and Hedeker, D. (2001) A Random-Effects Mixture Model for Classifying Treatment Response in Longitudinal Clinical Trials, *Journal of Biopharmaceutical Statistics*, **11(4)**, 253–273.

Young, D. S. and Hunter, D. R. (2015) Random Effects Regression Mixtures for Analyzing Infant Habituation, *Journal of Applied Statistics*, to appear.

#### See Also

```
regmixEM, post.beta
```

regmixMH 63

regmixMH

Metropolis-Hastings Algorithm for Mixtures of Regressions

# **Description**

Return Metropolis-Hastings (M-H) algorithm output for mixtures of multiple regressions with arbitrarily many components.

# Usage

```
regmixMH(y, x, lambda = NULL, beta = NULL, s = NULL, k = 2, addintercept = TRUE, mu = NULL, sig = NULL, lam.hyp = NULL, sampsize = 1000, omega = 0.01, thin = 1)
```

# **Arguments**

Samones	
У	An n-vector of response values.
X	An nxp matrix of predictors. See addintercept below.
lambda	Initial value of mixing proportions. Entries should sum to 1. This determines number of components. If NULL, then lambda is random from uniform Dirichlet and number of components is determined by beta.
beta	Initial value of beta parameters. Should be a pxk matrix, where p is the number of columns of x and k is number of components. If NULL, then beta has uniform standard normal entries. If both lambda and beta are NULL, then number of components is determined by s.
S	k-vector of standard deviations. If NULL, then $1/s^2$ has random standard exponential entries. If lambda, beta, and s are NULL, then number of components determined by k.
k	Number of components. Ignored unless all of lambda, beta, and s are NULL.
addintercept	If TRUE, a column of ones is appended to the x matrix before the value of p is calculated.
mu	The prior hyperparameter of same size as beta; the means of beta components. If NULL, these are set to zero.
sig	The prior hyperparameter of same size as beta; the standard deviations of beta components. If NULL, these are all set to five times the overall standard deviation of y.

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lam.hyp	The prior hyperparameter of length k for the mixing proportions (i.e., these are hyperparameters for the Dirichlet distribution). If NULL, these are generated from a standard uniform distribution and then scaled to sum to 1.
sampsize	Size of posterior sample returned.
omega	Multiplier of step size to control M-H acceptance rate. Values closer to zero result in higher acceptance rates, generally.
thin	Lag between parameter vectors that will be kept.

### Value

regmixMH returns a list of class mixMCMC with items:

x A nxp matrix of the predictors.

y A vector of the responses.

theta A (sampsize/thin) x q matrix of MCMC-sampled q-vectors, where q is the

total number of parameters in beta, s, and lambda.

k The number of components.

## References

Hurn, M., Justel, A. and Robert, C. P. (2003) Estimating Mixtures of Regressions, *Journal of Computational and Graphical Statistics* **12(1)**, 55–79.

# See Also

regcr

regmixmodel.sel 65

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Model Selection in Mixtures of Regressions

# Description

Assess the number of components in a mixture of regressions model using the Akaike's information criterion (AIC), Schwartz's Bayesian information criterion (BIC), Bozdogan's consistent AIC (CAIC), and Integrated Completed Likelihood (ICL).

## Usage

## **Arguments**

X	An nxp matrix (or list) of predictors. If an intercept is required, then x must NOT include a column of 1's! Requiring an intercept may be controlled through arguments specified in
у	An n-vector (or list) of response values.
W	An optional list of fixed effects predictors for type "mixed" or "random".
k	The maximum number of components to assess.
type	The type of regression mixture to use. If "fixed", then a mixture of regressions with fixed effects will be used. If "random", then a mixture of regressions where the random effects regression coefficients are assumed to come from a mixture will be used. If "mixed", the mixture structure used is the same as "random", except a coefficient of fixed effects is also assumed.
	Additional arguments passed to the EM algorithm used for calculating the type of regression mixture specified in type.

## Value

regmixmodel.sel returns a matrix of the AIC, BIC, CAIC, and ICL values along with the winner (i.e., the highest value given by the model selection criterion) for various types of regression mixtures.

# References

Biernacki, C., Celeux, G. and Govaert, G. (2000) Assessing a Mixture Model for Clustering with the Integrated Completed Likelihood, *IEEE Transactions on Pattern Analysis and Machine Intelligence* **22(7)**, 719–725.

Bozdogan, H. (1987) Model Selection and Akaike's Information Criterion (AIC): The General Theory and its Analytical Extensions, *Psychometrika* **52**, 345–370.

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## See Also

```
regmixEM, regmixEM.mixed
```

# **Examples**

```
## Assessing the number of components for NOdata.

data(NOdata)
attach(NOdata)
set.seed(100)
regmixmodel.sel(x = NO, y = Equivalence, k = 3, type = "fixed")
```

repnormmixEM

EM Algorithm for Mixtures of Normals with Repeated Measurements

# **Description**

Returns EM algorithm output for mixtures of normals with repeated measurements and arbitrarily many components.

# Usage

# **Arguments**

х	An mxn matrix of data. The columns correspond to the subjects and the rows correspond to the repeated measurements.
lambda	Initial value of mixing proportions. Entries should sum to 1. This determines number of components. If NULL, then lambda is random from uniform Dirichlet and number of components is determined by mu.
mu	A k-vector of component means. If NULL, then mu is determined by a normal distribution according to a binning method done on the data. If both lambda and mu are NULL, then number of components is determined by sigma.
sigma	A vector of standard deviations. If NULL, then 1/sigma <sup>2</sup> has random standard exponential entries according to a binning method done on the data. If lambda, mu, and sigma are NULL, then number of components is determined by k.
k	Number of components. Ignored unless all of lambda, mu, and sigma are NULL.
arbmean	If TRUE, then the component densities are allowed to have different mus. If FALSE, then a scale mixture will be fit.
arbvar	If TRUE, then the component densities are allowed to have different sigmas. If FALSE, then a location mixture will be fit.
epsilon	The convergence criterion.
maxit	The maximum number of iterations.
verb	If TRUE, then various updates are printed during each iteration of the algorithm.

repnormmixmodel.sel 67

### Value

repnormmixEM returns a list of class mixEM with items:

The raw data.

The final mixing proportions.
 The final mean parameters.
 Sigma The final standard deviations. If arbmean = FALSE, then only the smallest standard deviation is returned. See scale below.
 If arbmean = FALSE, then the scale factor for the component standard deviations is returned. Otherwise, this is omitted from the output.
 The final log-likelihood.
 An nxk matrix of posterior probabilities for observations.

poster for An lixk matrix of posterior probabilities for observations.

all.loglik A vector of each iteration's log-likelihood.

restarts The number of times the algorithm restarted due to unacceptable choice of initial

values.

ft A character vector giving the name of the function.

### References

Hettmansperger, T. P. and Thomas, H. (2000) Almost Nonparametric Inference for Repeated Measures in Mixture Models, *Journal of the Royals Statistical Society, Series B* **62(4)** 811–825.

## See Also

normalmixEM

# **Examples**

```
## EM output for the water-level task data set.

data(Waterdata)
set.seed(100)
water <- t(as.matrix(Waterdata[,3:10]))
em.out <- repnormmixEM(water, k = 2, verb = TRUE, epsilon = 1e-03)
em.out</pre>
```

repnormmixmodel.sel

Model Selection in Mixtures of Normals with Repeated Measures

# **Description**

Assess the number of components in a mixture model with normal components and repeated measures using the Akaike's information criterion (AIC), Schwartz's Bayesian information criterion (BIC), Bozdogan's consistent AIC (CAIC), and Integrated Completed Likelihood (ICL).

68 rmvnorm

## Usage

```
repnormmixmodel.sel(x, k = 2, ...)
```

## **Arguments**

An mxn matrix of observations. The rows correspond to the repeated measures and the columns correspond to the subject.

k The maximum number of components to assess.

... Additional arguments passed to repnormmixEM.

### Value

repnormmixmodel.sel returns a matrix of the AIC, BIC, CAIC, and ICL values along with the winner (i.e., the highest value given by the model selection criterion) for a mixture of normals with repeated measures.

### References

Biernacki, C., Celeux, G., and Govaert, G. (2000). Assessing a Mixture Model for Clustering with the Integrated Completed Likelihood. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 22(7):719-725.

Bozdogan, H. (1987). Model Selection and Akaike's Information Criterion (AIC): The General Theory and its Analytical Extensions. *Psychometrika*, 52:345-370.

## See Also

repnormmixEM

### **Examples**

```
## Assessing the number of components for the water-level task data set.
data(Waterdata)
water<-t(as.matrix(Waterdata[,3:10]))
set.seed(100)
out <- repnormmixmodel.sel(water, k = 3, epsilon = 1e-01)
out</pre>
```

rmvnorm

Simulate from a Multivariate Normal Distribution

# **Description**

Simulate from a multiviate normal distribution

```
rmvnorm(n, mu=NULL, sigma=NULL)
```

rmvnormmix 69

## **Arguments**

n Number of vectors to simulate

mu mean vector

sigma covariance matrix, assumed symmetric and nonnegative definite

#### **Details**

This function uses an eigen decomposition assuming sigma is symmetric. In particular, the upper triangle of sigma is ignored.

## Value

An  $n \times d$  matrix in which each row is an independently generated realization from the desired multivariate normal distribution

## See Also

eigen, dnorm, dmvnorm

rmvnormmix

Simulate from Multivariate (repeated measures) Mixtures of Normals

# **Description**

Simulate from a mixture of multivariate zero-correlation normal distributions

### **Usage**

```
rmvnormmix(n, lambda=1, mu=0, sigma=1)
```

# **Arguments**

n Number of cases to simulate.

lambda Vector of mixture probabilities with length equal to m, the desired number of

components. This is assumed to sum to 1; if not, it is normalized.

mu Matrix of means of dimensions  $m \times r$ , where m is the number of components

(subpopulations) and r is the number of coordinates (repeated measurements) per case. Note: mu is automatically coerced to a matrix with m rows even if it is not given in this form, which can lead to unexpected behavior in some cases.

sigma Matrix of standard deviations, same dimensions as mu. The coordinates within a

case are independent, conditional on the mixture component. (There is marginal correlation among the coordinates, but this is due to the mixture structure only.) Note: sigma is automatically coerced to a matrix with m rows even if it is not given in this form, which can lead to unexpected behavior in some cases.

70 rnormmix

## **Details**

It is possible to generate univariate standard normal random variables using the default values (but why bother?). The case of conditionally iid coordinates is covered by the situation in which all columns in mu and sigma are identical.

#### Value

rmvnormmix returns an  $n \times r$  matrix in which each row is a sample from one of the components of a mixture of zero-correlation multivariate normals. The mixture structure induces nonzero correlations among the coordinates.

## See Also

rnormmix

# **Examples**

rnormmix

Simulate from Mixtures of Normals

# Description

Simulate from a mixture of univariate normal distributions.

# Usage

```
rnormmix(n, lambda=1, mu=0, sigma=1)
```

## **Arguments**

n

Number of cases to simulate.

lambda

Vector of mixture probabilities, with length equal to m, the desired number of components (subpopulations). This is assumed to sum to 1; if not, it is normalized.

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mu Vector of means.

sigma Vector of standard deviations.

### **Details**

This function simply calls rmvnormmix.

## Value

rnormmix returns an n-vector sampled from an m-component mixture of univariate normal distributions.

## See Also

```
makemultdata, rmvnormmix
```

# **Examples**

```
##Generate data from a 2-component mixture of normals.
set.seed(100)
n <- 500
lambda <- rep(1, 2)/2
mu <- c(0, 5)
sigma <- rep(1, 2)
mixnorm.data <- rnormmix(n, lambda, mu, sigma)
##A histogram of the simulated data.
hist(mixnorm.data)</pre>
```

RodFramedata

Rod and Frame Task Data Set

# **Description**

This data set involves assessing children longitudinally at 6 age points from ages 4 through 18 years for the rod and frame task. This task sits the child in a darkened room in front of a luminous square frame tilted at 28 degrees on its axis to the left or right. Centered inside the frame was a luminous rod also tilted 28 degrees to the left or right. The child's task was to adjust the rod to the vertical position and the absolute deviation from the vertical (in degrees) was the measured response.

# Usage

RodFramedata

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### **Format**

This data frame consists of 140 children (the rows). Column 1 is the subject number and column 2 is the sex (0=MALE and 1=FEMALE). Columns 3 through 26 give the 8 responses at each of the ages 4, 5, and 7. Columns 27 through 56 give the 10 responses at each of the ages 11, 14, and 18. A value of 99 denotes missing data.

#### Source

Thomas, H. and Dahlin, M. P. (2005) Individual Development and Latent Groups: Analytical Tools for Interpreting Heterogeneity, *Developmental Review* **25(2)**, 133–154.

RTdata

Reaction Time (RT) Data Set

# **Description**

This data set involves normally developing children 9 years of age presented with two visual simuli on a computer monitor. The left image is the target stimuli and on the right is either an exact copy or a mirror image of the target stimuli. The child must press one key if it is a copy or another key if it is a mirror image. The data consists of the reaction times (RT) of the 197 children who provided correct responses for all 6 task trials.

# Usage

RTdata

### **Format**

This data frame consists of 197 children (the rows) and their 6 responses (the columns) to the stimulus presented. The response (RT) is recorded in milliseconds.

### References

Cruz-Medina, I. R., Hettmansperger, T. P. and Thomas, H. (2004) Semiparametric Mixture Models and Repeated Measures: The Multinomial Cut Point Model, *Applied Statistics* **53**(3), 463–474.

Miller, C. A., Kail, R., Leonard, L. B. and Tomblin, J. B. (2001) Speed of Processing in Children with Specific Language Impairment, *Journal of Speech, Language, and Hearing Research* **44(2)**, 416–433.

### See Also

RTdata2

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RTdata2

Reaction Time (RT) Data Set \# 2

# **Description**

This data set involves normally developing children 9 years of age presented visual simuli on a computer monitor. There are three different experimental conditions, according to the length of the delay after which the stimulus was displayed on the screen. Each subject experienced each condition eight times, and these 24 trials were given in random order. These data give the 82 children for whom there are complete measurements among over 200 total subjects.

## Usage

RTdata2

#### **Format**

This data frame consists of 82 children (the rows) and their 24 responses (the columns) to the stimulus presented. The response is recorded in milliseconds. The columns are not in the order in which the stimuli were presented to the children; rather, they are arranged into three blocks of eight columns each so that each eight-column block contains only trials from one of the three conditions.

# References

Miller, C. A., Kail, R., Leonard, L. B. and Tomblin, J. B. (2001) Speed of Processing in Children with Specific Language Impairment, *Journal of Speech, Language, and Hearing Research* **44(2)**, 416–433.

#### See Also

**RTdata** 

segregmixEM

ECM Algorithm for Mixtures of Regressions with Changepoints

#### **Description**

Returns ECM algorithm output for mixtures of multiple regressions with changepoints and arbitrarily many components.

# Usage

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#### **Arguments**

An n-vector of response values. У An nxp matrix of predictors. Note that this model assumes the presence of an Х intercept. lambda Initial value of mixing proportions. Entries should sum to 1. This determines number of components. If NULL, then lambda is random from uniform Dirichlet and the number of components is determined by beta. beta Initial value of beta parameters. This is a list of length k such that each element must contain a vector having length consistent with the defined changepoint structure. See seg. Z, psi, and psi. loc below. If NULL, then beta has standard normal entries according to a binning method done on the data. If both lambda and beta are NULL, then number of components is determined by sigma. A vector of standard deviations. If NULL, then 1/sigma^2 has random standard sigma exponential entries according to a binning method done on the data. If lambda, beta, and sigma are NULL, then number of components is determined by k. k Number of components. Ignored unless all of lambda, beta, and sigma are NULL. seg.Z A list of length k whose elements are right-hand side formulas, which are additive linear models of the predictors that have changepoints in their respective components. See below for more details. psi A kxp matrix specifying the number of changepoints for each predictor in each component. See below for more details. psi.locs A list of length k that has initial estimates for the changepoint locations. Each element of the list must have length equal to the number of chanegpoints specified in the corresponding row of the psi matrix. For components with no changepoints, simply set that element equal to NULL. See below for more details. delta An optional list of values quantifying the amount of separation at each changepoint if assuming discontinuities at the changepoints. This has the same dimensions as psi.locs. epsilon The convergence criterion. The maximum number of iterations. maxit If TRUE, then various updates are printed during each iteration of the algorithm. verb The number of times to try restarting the ECM algorithm if estimation problems max.restarts occur - such as choice of poor initial values or a poorly chosen changepoint

#### Details

structure.

seg.Z is defined as a list of right-hand side linear model formulas that are used to identify which predictors have changepoints in each component. For example, suppose you have a dataframe with three predictors: V1, V2, V3. Suppose now that you wish to model a 3-component mixture of regressions with changepoints structure such that the first component has changepoints in V1 and V2, the second component has changepoints in V3, and the third component has no changepoints. Then you would define seg.Z = list(~V1+V2, ~V3, NULL). Note that you MUST place the variables in order with respect to how they appear in the predictor matrix x.

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psi is a kxp matrix specifying the number of changepoints for each predictor in each component. For the example given above, suppose there are three changepoints for V1, two changepoints for V2, and four changepoints for V3. Then you would define psi = rbind(c(3, 2, 0), c(0, 0, 4), c(0, 0, 0)).

psi.locs is a list of length k whose elements give the initial locations of the changepoints for each component. Each element of the list must have length equal to the total number of changepoints for that component's regression equation. For the example given above, in component 1, assume that the three changepoints for V1 are at 3, 7, and 10 and the two changepoints for V1 are at 5, 20, and 30. In component 2, assume that the four changepoints for V3 are at 2, 4, 6, and 8. Then you would define psi.locs = list(c(3, 7, 10, 5, 20, 30), c(2, 4, 6, 8), NULL). Note that the order of the changepoints is determined by first sorting the predictors by how they appear in the formulas in seg. Z and then sorting in increasing order within each predictor.

#### Value

segregmixEM returns a list of class segregmixEM with items:

x The set of predictors.y The response values.

lambda The final mixing proportions.beta The final regression coefficients.sigma The final standard deviations.

seg. Z The list of right-hand side formulas as defined by the user.

psi.locs A list of length k with the final estimates for the changepoint locations.

delta A list of the delta values that were optionally specified by the user.

loglik The final log-likelihood.

posterior An nxk matrix of posterior probabilities for observations.

all.loglik A vector of each iteration's log-likelihood.

restarts The number of times the algorithm restarted due to unacceptable choice of initial

values.

ft A character vector giving the name of the function.

#### Note

As of version 0.4.6, this more general function has replaced the now defunct regmixEM. chgpt and associated internal functions.

## References

Young, D. S. (2014) Mixtures of Regressions with Changepoints, *Statistics and Computing*, **24(2)**, 265–281.

# See Also

regmixEM

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## **Examples**

```
## Not run:
## Simulated example.
set.seed(100)
x <- 1:20
y1 < -3 + x + rnorm(20)
y2 < -3 - x - 5*(x - 15)*(x > 15) + rnorm(20)
y < -c(y1, y2)
x \leftarrow c(x, x)
set.seed(100)
be \leftarrow list(c(3, -1, -5), c(3, 1))
s \leftarrow c(1, 1)
psi.locs \leftarrow list(comp.1 = list(x = 15), comp.2 = NULL)
out <- segregmixEM(y, cbind(1,x), verb = TRUE, k = 2,
                    beta = be, sigma = s, lambda = c(1, 1)/2,
                    seg.Z = list(\sim x, NULL), psi = rbind(1, 0),
                    psi.locs = psi.locs, epsilon = 0.9)
z < - seq(0, 21, len = 40)
plot(x, y, col = apply(out$post, 1, which.max) + 1, pch = 19,
   cex.lab = 1.4, cex = 1.4)
b <- out$beta
d <- out$psi.locs</pre>
lines(z, b[[1]][1] + b[[1]][2] * z + b[[1]][3] *
      (z - d[[1]][[1]]) * (z > d[[1]][[1]]) , col = 2, lwd = 2)
lines(z, b[[2]][1] + b[[2]][2] * z, col = 3, lwd = 2)
abline(v = outspsi.locs[[1]][1], col = 2, lty = 2)
## End(Not run)
## Not run:
## Example using the NOdata.
data(NOdata)
attach(NOdata)
set.seed(100)
be \leftarrow list(c(1.30, -0.13, 0.08), c(0.56, 0.09))
s < -c(0.02, 0.04)
psi.locs <- list(comp.1 = list(NO = 1.57), comp.2 = NULL)</pre>
out <- segregmixEM(Equivalence, cbind(NO), verb = TRUE, k = 2,
                    beta = be, sigma = s, lambda = c(1, 1)/2,
                    seg.Z = list(\sim NO, NULL), psi = rbind(1, 0),
                    psi.locs = psi.locs, epsilon = 0.1)
z < - seq(0, 5, len = 1000)
plot(NOdata, col = apply(out$post, 1, which.max) + 1, pch = 19,
   cex.lab = 1.4, cex = 1.4, ylab = "Equivalence Ratio")
b <- out$beta
d <- out$psi.locs</pre>
```

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spEM

Semiparametric EM-like Algorithm for Mixtures of Independent Repeated Measurements

## **Description**

Returns semiparametric EM algorithm output (Benaglia et al, 2009) for mixtures of multivariate (repeated measures) data where the coordinates of a row (case) in the data matrix are assumed to be independent, conditional on the mixture component (subpopulation) from which they are drawn. For now, this algorithm only implements model (4.7) in Benaglia et al, in which each component and block has exactly the same (nonparametric) shape and they differ only by location and scale.

## Usage

```
spEM(x, mu0, blockid = 1:ncol(x),
    bw = bw.nrd0(as.vector(as.matrix(x))), constbw = TRUE,
    h = bw, eps = 1e-8,
    maxiter = 500, stochastic = FALSE, verb = TRUE)
```

# **Arguments**

Х

An  $n \times r$  matrix of data. Each of the n rows is a case, and each case has r repeated measurements. These measurements are assumed to be conditionally independent, conditional on the mixture component (subpopulation) from which the case is drawn.

mu0

Either an  $m \times r$  matrix specifying the initial centers for the kmeans function, or an integer m specifying the number of initial centers, which are then choosen randomly in kmeans

blockid

A vector of length r identifying coordinates (columns of x) that are assumed to be identically distributed (i.e., in the same block). For instance, the default has all distinct elements, indicating that no two coordinates are assumed identically distributed and thus a separate set of m density estimates is produced for each column of x. On the other hand, if blockid=rep(1,ncol(x)), then the coordinates in each row are assumed conditionally i.i.d.

bw

Bandwidth for density estimation, equal to the standard deviation of the kernel density. By default, a simplistic application of the default bw.nrd0 bandwidth used by density to the entire dataset.

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constbw Logical: If TRUE, use the same bandwidth for each iteration and for each com-

ponent and block. If FALSE, use a separate bandwidth for each component and block, and update this bandwidth at each iteration of the algorithm using a suit-

ably modified bw.nrd0 method as described in Benaglia et al (2011).

h Alternative way to specify the bandwidth, to provide backward compatibility.

eps Tolerance limit for declaring algorithm convergence. Convergence is declared

whenever the maximum change in any coordinate of the lambda vector (of mix-

ing proportion estimates) does not exceed eps.

maxiter The maximum number of iterations allowed, for both stochastic and non-stochastic

versions; for non-stochastic algorithms (stochastic = FALSE), convergence

may be declared before maxiter iterations (see eps above).

stochastic Flag, if FALSE (the default), runs the non-stochastic version of the npEM algo-

rithm, as in Benaglia et al (2009). Set to TRUE to run a stochastic version which simulates the posteriors at each iteration, and runs for maxiter iterations.

verb If TRUE, print updates for every iteration of the algorithm as it runs

#### Value

spEM returns a list of class spEM with the following items:

data The raw data (an  $n \times r$  matrix).

posteriors An  $n \times m$  matrix of posterior probabilities for observation. If stochastic = TRUE,

this matrix is computed from an average over the maxiter iterations.

bandwidth If constbw==TRUE, same as the bw input argument; otherwise, value of bw matrix

at final iteration (since for now this algorithm only implements model (4.7) in Benaglia et al, the bandwidth matrix is reduced to a single bandwith scalar). This information is needed by any method that produces density estimates from

the output.

blockid Same as the blockid input argument, but recoded to have positive integer val-

ues. Also needed by any method that produces density estimates from the out-

put.

lambda The sequence of mixing proportions over iterations.

lambdahat The final mixing proportions if stochastic = FALSE, or the average mixing

proportions if stochastic = TRUE.

mu The sequence of location parameters over iterations.

muhat The final location parameters if stochastic = FALSE, or the average location

parameters if stochastic = TRUE.

sigma The sequence of scale parameters over iterations.

sigmahat The final scale parameters if stochastic = FALSE, or the average scale param-

eters if stochastic = TRUE.

loglik The sequence of log-likelihoods over iterations.

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#### References

 Benaglia, T., Chauveau, D., and Hunter, D. R., An EM-like algorithm for semi- and nonparametric estimation in multivariate mixtures, Journal of Computational and Graphical Statistics, 18, 505-526, 2009.

- Benaglia, T., Chauveau, D. and Hunter, D.R. Bandwidth Selection in an EM-like algorithm for nonparametric multivariate mixtures. Nonparametric Statistics and Mixture Models: A Festschrift in Honor of Thomas P. Hettmansperger. World Scientific Publishing Co., pages 15-27, 2011.
- Bordes, L., Chauveau, D., and Vandekerkhove, P., An EM algorithm for a semiparametric mixture model, Computational Statistics and Data Analysis, 51: 5429-5443, 2007.

#### See Also

```
plot.spEM, normmixrm.sim, spEMsymloc, npEM, plotseq.npEM
```

# **Examples**

spEMsymloc

Semiparametric EM-like Algorithm for univariate symmetric location mixture

# **Description**

Returns semiparametric EM algorithm output (Bordes et al, 2007, and Benaglia et al, 2009) for location mixtures of univariate data and symmetric component density.

## Usage

```
spEMsymloc(x, mu0, bw = bw.nrd0(x), h=bw, eps = 1e-8, maxiter = 100,
    stochastic = FALSE, verbose = FALSE)
```

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#### **Arguments**

A vector of length n consisting of the data. Х mu0 Either a vector specifying the initial centers for the kmeans function, and from which the number of component is obtained, or an integer m specifying the number of initial centers, which are then choosen randomly in kmeans. bw Bandwidth for density estimation, equal to the standard deviation of the kernel density. h Alternative way to specify the bandwidth, to provide backward compatibility. Tolerance limit for declaring algorithm convergence. Convergence is declared eps before maxiter iterations whenever the maximum change in any coordinate of the lambda (mixing proportion estimates) and mu (means) vector does not exceed eps. maxiter The maximum number of iterations allowed, for both stochastic and non-stochastic versions; for non-stochastic algorithms (stochastic = FALSE), convergence may be declared before maxiter iterations (see eps above). stochastic Flag, if FALSE (the default), runs the non-stochastic version of the algorithm, as in Benaglia et al (2009). Set to TRUE to run a stochastic version which simulates the posteriors at each iteration (as in Bordes et al, 2007), and runs for maxiter iterations. verbose If TRUE, print updates for every iteration of the algorithm as it runs

#### Value

spEMsymloc returns a list of class npEM with the following items:

data The raw data (an  $n \times r$  matrix). posteriors An  $n \times m$  matrix of posterior probabilities for observations. If stochastic = TRUE, this matrix is computed from an average over the maxiter iterations. bandwidth Same as the bw input argument, returned because this information is needed by any method that produces density estimates from the output. lambda The sequence of mixing proportions over iterations. lambdahat The final estimate for mixing proportions if stochastic = FALSE, the average over the sequence if stochastic = TRUE. the sequence of component means over iterations. mu muhat the final estimate of component means if stochastic = FALSE, the average over the sequence if stochastic = TRUE. Flag indicating that the kernel density estimate is using a symmetry assumption. symmetric

#### References

- Benaglia, T., Chauveau, D., and Hunter, D. R., An EM-like algorithm for semi- and nonparametric estimation in multivariate mixtures, Journal of Computational and Graphical Statistics, 18, 505-526, 2009.
- Benaglia, T., Chauveau, D., Hunter, D. R., and Young, D. mixtools: An R package for analyzing finite mixture models. Journal of Statistical Software, 32(6):1-29, 2009.

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• Bordes, L., Chauveau, D., and Vandekerkhove, P. (2007), An EM algorithm for a semiparametric mixture model, Computational Statistics and Data Analysis, 51: 5429-5443.

# See Also

```
plot.npEM, rnormmix, npEM, spEMsymlocN01, plotseq.npEM
```

# **Examples**

```
## Example from a normal location mixture set.seed(100) n <- 200 lambda <- c(1/3,2/3) mu <- c(0, 4); sigma<-rep(1, 2) x <- rnormmix(n, lambda, mu, sigma) out.stoc <- spEMsymloc(x, mu0=c(-1, 2), stochastic=TRUE) out.nonstoc <- spEMsymloc(x, mu0=c(-1, 2))
```

spEMsymlocN01

semiparametric EM-like algorithm for univariate mixture in False Discovery Rate (FDR) estimation

# **Description**

Return semiparametric EM-like algorithm output for a 2-components mixture model with one component set to Normal(0,1), and the other component being a unspecified but symmetric density with a location parameter. This model is tailored to FDR estimation on probit transform (qnorm) of p-values arising from multiple testing.

# Usage

```
spEMsymlocN01 (x, mu0 = 2, bw = bw.nrd0(x), h=bw, eps = 1e-8, maxiter = 100, verbose = FALSE, plotf = FALSE)
```

## **Arguments**

X	A vector of length n consisting of the data, probit transform of pvalues, preferably sorted.
mu0	Starting value of vector of component means. If not set then the initial value is randomly generated by a kmeans of the data in two bins. Since component 1 is theoretically normal(0,1), mu[1] must be 0 and mu[2] some negative value (see details).
bw	Bandwidth for weighted kernel density estimation.
h	Alternative way to specify the bandwidth, to provide backward compatibility.
eps	Tolerance limit for declaring algorithm convergence. Convergence is declared before maxiter iterations whenever the maximum change in any coordinate of the lambda (mixing proportion estimates) and mu (mean of the semiparametric component) vector does not exceed eps

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maxiter The maximum number of iterations allowed; convergence may be declared be-

fore maxiter iterations (see eps above).

verbose If TRUE, print updates for every iteration of the algorithm as it runs.

plotf If TRUE, plots successive updates of the nonparametric density estimate over

iterations. Mostly for testing purpose.

#### **Details**

This algorithm is a specific version of semiparametric EM-like algorithm similar in spirit to spEMsymloc, but specialized for FDR estimation on probit transform (qnorm) of p-values in multiple testing framework. In this model, component 1 corresponds to the individuals under the null hypothesis, i.e. theoretically normal(0,1) distributed, whereas component 2 corresponds to individuals in the alternative hypothesis, with typically very small p-values and consequently negative values for probit(p) data. This model only assumes that these individuals come from an unspecified but symmetric density with a location parameter, as in Bordes and Vandekerkhove (2010) and Chauveau et al. (2014).

#### Value

spEMsymlocN01 returns a list of class spEMN01 with the following items:

data The raw data (an  $n \times r$  matrix).

posteriors An  $n \times 2$  matrix of posterior probabilities for observations. This can be used in,

e.g., plotFDR to plot False Discovery Rate estimates.

bandwidth Same as the bw input argument, returned because this information is needed by

any method that produces density estimates from the output.

lambda The sequence of mixing proportions over iterations.

lambdahat The final estimate for mixing proportions.

mu the sequence of second component mean over iterations.

muhat the final estimate of second component mean.

symmetric Flag indicating that the kernel density estimate is using a symmetry assumption.

#### Author(s)

Didier Chauveau

## References

- Bordes, L. and Vandekerkhove, P. (2010). Semiparametric two-component mixture model with a known component: an asymptotically normal estimator. Mathematical Methods of Statistics, 19(1):22-41
- Chauveau, D., Saby, N., Orton, T. G., Lemercier B., Walter, C. and Arrouys, D. (2014) Large-scale simultaneous hypothesis testing in monitoring carbon content from french soil database: A semi-parametric mixture approach. Geoderma 219-220 (2014): 117-124.

#### See Also

spEMsymloc, normalmixEM, npEM, plot.spEMN01, plotFDR

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# **Examples**

```
## Probit transform of p-values
## from a Beta-Uniform mixture model
## comparion of parametric and semiparametric EM fit
## Note: in actual situations n=thousands
set.seed(50)
n=300 # nb of multiple tests
m=2 # 2 mixture components
a=c(1,0.1); b=c(1,1); lambda=c(0.6,0.4) # parameters
z=sample(1:m, n, rep=TRUE, prob = lambda)
p < - rbeta(n, shape1 = a[z], shape2 = b[z]) # p-values
o <- order(p)</pre>
cpd <- cbind(z,p)[o,] # sorted complete data, z=1 if H0, 2 if H1</pre>
p <- cpd[,2] # sorted p-values</pre>
y <- qnorm(p) # probit transform of the pvalues
# gaussian EM fit with component 1 constrained to N(0,1)
s1 <- normalmixEM(y, mu=c(0,-4),
mean.constr = c(0,NA), sd.constr = c(1,NA))
s2 <- spEMsymlocN01(y, mu0 = c(0,-3)) # spEM with N(0,1) fit
hist(y, freq = FALSE, col = 8, main = "histogram of probit(pvalues)")
plot(s2, add.plot = TRUE, lwd = 2)
# Exemples of plot capabilities
# Note: posteriors must be ordered by p for plot.FDR
# plotFDR(s1$post) # when true complete data not observed
# plotFDR(s1$post, s2$post) # comparing 2 strategies
plotFDR(s1$post, s2$post, lg1 = "normalmixEM", lg2 = "spEMsymlocN01",
complete.data = cpd) \# with true FDR computed from z
```

spregmix

EM-like Algorithm for Semiparametric Mixtures of Regressions

# Description

Returns parameter estimates for finite mixtures of linear regressions with unspecified error structure. Based on Hunter and Young (2012).

#### **Usage**

```
spregmix(lmformula, bw = NULL, constbw = FALSE,
    bwmult = 0.9, z.hat = NULL, symm = TRUE, betamethod = "LS",
    m = ifelse(is.null(z.hat), 2, ncol(z.hat)),
    epsilon = 1e-04, maxit = 1000, verbose = FALSE,
    ...)
```

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#### **Arguments**

1mformula Formula for a linear model, in the same format used by 1m. Additional parameters may be passed to 1m via the . . . argument. bw

Initial bandwidth value. If NULL, this will be chosen automatically by the al-

gorithm.

constbw Logical: If TRUE, the bandwidth is held constant throughout the algorithm; if

FALSE, it adapts at each iteration according to the rules given in Hunter and

Young (2012).

bwmult Whenever it is updated automatically, the bandwidth is equal to bwmult divided

> by the fifth root of n times the smaller of s and IQR/1.34, where s and IQR are estimates of the standard deviation and interquartile range of the residuals, as explained in Hunter and Young (2012). The value of 0.9 gives the rule of Silverman (1986) and the value of 1.06 gives the rule of Scott (1992). Larger values lead to greater smoothing, whereas smaller values lead to less smoothing.

z.hat Initial nxm matrix of posterior probabilities. If NULL, this is initialized ran-

> domly. As long as a parametric estimation method like least squares is used to estimate beta in each M-step, the z. hat values are the only values necessary to

begin the EM iterations.

Logical: If TRUE, the error density is assumed symmetric about zero. If FALSE, symm

it is not. WARNING: If FALSE, the intercept parameter is not uniquely identi-

fiable if it is included in the linear model.

betamethod Method of calculating beta coefficients in the M-step. Current possible val-

> ues are "LS" for least-squares; "L1" for least absolute deviation; "NP" for fully nonparametric; and "transition" for a transition from least squares to fully nonparametric. If something other than these four possibilities is used, then "NP" is

assumed. For details of these methods, see Hunter and Young (2012).

Number of components in the mixture.

epsilon Convergence is declared if the largest change in any lambda or beta coordinate

is smaller than epsilon.

maxit The maximum number of iterations; if convergence is never declared based on

comparison with epsilon, then the algorithm stops after maxit iterations.

Logical: If TRUE, then various updates are printed during each iteration of the verbose

algorithm.

Additional parameters passed to the model. frame and model. matrix functions,

which are used to obtain the response and predictor of the regression.

# Value

regmixEM returns a list of class npEM with items:

The set of predictors (which includes a column of 1's if addintercept = TRUE).

The response values. у

lambda The mixing proportions for every iteration in the form of a matrix with m columns

and (#iterations) rows

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beta	The final regression coefficients.
posterior	An nxm matrix of posterior probabilities for observations.
np.stdev	Nonparametric estimate of the standard deviation, as given in Hunter and Young $(2012)$
bandwidth	Final value of the bandwidth
density.x	Points at which the error density is estimated
density.y	Values of the error density at the points density.x
symmetric	Logical: Was the error density assumed symmetric?
loglik	A quantity similar to a log-likelihood, computed just like a standard loglikelihood would be, conditional on the component density functions being equal to the final density estimates.
ft	A character vector giving the name of the function.

## References

Hunter, D. R. and Young, D. S. (2012) Semi-parametric Mixtures of Regressions, Journal of Nonparametric Statistics 24(1): 19-38.

Scott, D. W. (1992) Multivariate Density Estimation, John Wiley & Sons Inc., New York.

Silverman, B. W. (1986). Density Estimation for Statistics and Data Analysis, Chapman & Hall, London.

## See Also

```
regmixEM, spEMsymloc, lm
```

# **Examples**

```
data(tonedata)
## By default, the bandwidth will adapt and the error density is assumed symmetric
set.seed(100)
a=spregmix(tuned~stretchratio, bw=.2, data=tonedata, verb=TRUE)
## Look at the sp mixreg solution:
plot(tonedata)
abline(a=a$beta[1,1],b=a$beta[2,1], col=2)
abline(a=a$beta[1,2],b=a$beta[2,2], col=3)
## Look at the nonparametric KD-based estimate of the error density,
## constrained to be zero-symmetric:
plot(xx<-a$density.x, yy<-a$density.y, type="1")</pre>
## Compare to a normal density with mean 0 and NP-estimated stdev:
z \leftarrow seq(min(xx), max(xx), len=200)
lines(z, dnorm(z, sd=sqrt((a$np.stdev)^2+a$bandwidth^2)), col=2, lty=2)
# Add bandwidth^2 to variance estimate to get estimated var of KDE
## Now add the sp mixreg estimate without assuming symmetric errors:
b=spregmix(tuned~stretchratio, bw=.2, , symm=FALSE, data=tonedata, verb=TRUE)
lines(b$density.x, b$density.y, col=3)
```

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summary	

Summarizing EM mixture model fits

# Description

summary method for class mixEM.

## Usage

```
## S3 method for class 'mixEM'
summary(object, digits=6, ...)
```

# **Arguments**

object an object of class mixEM such as a result of a call to normalmixEM

digits Significant digits for printing values

... further arguments passed to print method.

#### **Details**

summary.mixEM prints parameter estimates for each component of a fitted mixture model. The estimates printed vary with the type of model.

# Value

The function summary.mixEM prints the final loglikelihood value at the solution as well as a matrix of values for each component that could include:

lambdaThe estimated mixing weightsmuThe estimated mean parameterssigmaThe estimated standard deviationsthetaThe estimated multinomial parametersbetaThe estimated regression parameters

# See Also

normalmixEM, logisregmixEM, multmixEM, mvnormalmixEM, poisregmixEM, regmixEM. lambda, regmixEM.loc, regmixEM.mixed, regmixEM.chgpt, repnormmixEM

# **Examples**

```
data(faithful)
attach(faithful)
set.seed(100)
out <- normalmixEM(waiting, mu=c(50,80), sigma=c(5,5), lambda=c(.5,.5))
summary(out)</pre>
```

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summary.npEM	Summarizing non- and semi-parametric multivariate mixture model fits
	Jus

## **Description**

summary method for class npEM.

# Usage

```
## S3 method for class 'npEM'
summary(object, ...)
## S3 method for class 'summary.npEM'
print(x, digits=3, ...)
```

## **Arguments**

object, x an object of class npEM such as a result of a call to npEM digits Significant digits for printing values ... further arguments passed to or from other methods.

#### **Details**

summary.npEM prints means and variances of each block for each component. These quantities might not be part of the model, but they are estimated nonparametrically based on the posterior probabilities and the data.

# Value

The function summary.npEM returns a list of type summary.npEM with the following components:

n The number of observations

m The number of mixture components

B The number of blocks

blockid The block ID (from 1 through B) for each of the coordinates of the multivariate observations. The blockid component is of length r, the dimension of each observation.

means  $A B \times m$  matrix giving the estimated mean of each block in each component. variances Same as means but giving the estimated variances instead.

#### References

• Benaglia, T., Chauveau, D., and Hunter, D. R. (2009), An EM-like algorithm for semi- and non-parametric estimation in multivariate mixtures, Journal of Computational and Graphical Statistics (to appear).

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## See Also

```
npEM, plot.npEM
```

# **Examples**

```
data(Waterdata)
set.seed(100)
## Not run:
a <- npEM(Waterdata[,3:10], 3, bw=4) # Assume indep but not iid
summary(a)
b <- npEM(Waterdata[,3:10], 3, bw=4, blockid=rep(1,8)) # Now assume iid
summary(b)
## End(Not run)</pre>
```

test.equality

Performs Chi-Square Tests for Scale and Location Mixtures

## **Description**

Performs a likelihood ratio test of a location (or scale) normal or regression mixture versus the more general model. For a normal mixture, the alternative hypothesis is that each component has its own mean and variance, whereas the null is that all means (in the case of a scale mixture) or all variances (in the case of a location mixture) are equal. This test is asymptotically chi-square with degrees of freedom equal to k-1, where k is the number of components.

# Usage

# **Arguments**

У	The responses for regmixEM or the data for normalmixEM.
X	The predictors for regmixEM.
arbmean	$If \ FALSE, then \ a \ scale \ mixture \ analysis \ is \ performed \ for \ normal mixEM \ or \ regmixEM.$
arbvar	If FALSE, then a location mixture analysis is performed for normalmixEM or regmixEM.
mu	An optional vector for starting values (under the null hypothesis) for mu in normalmixEM.
sigma	An optional vector for starting values (under the null hypothesis) for sigma in normalmixEM or regmixEM.
beta	An optional matrix for starting values (under the null hypothesis) for beta in regmixEM.

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lambda	An otional vector for starting values (under the null hypothesis) for lambda in normalmixEM or regmixEM.
	Additional arguments passed to the various EM algorithms for the mixture of interest.

## Value

test.equality returns a list with the following items:

chi.sq The chi-squared test statistic.

df The degrees of freedom for the chi-squared test statistic.

p.value The p-value corresponding to this likelihood ratio test.

## See Also

```
test.equality.mixed
```

## **Examples**

```
## Should a location mixture be used for the Old Faithful data?

data(faithful)
attach(faithful)
set.seed(100)
test.equality(y = waiting, arbmean = FALSE, arbvar = TRUE)
```

test.equality.mixed

Performs Chi-Square Test for Mixed Effects Mixtures

# Description

Performs a likelihood ratio test of either common variance terms between the response trajectories in a mixture of random (or mixed) effects regressions or for common variance-covariance matrices for the random effects mixture distribution.

# Usage

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# **Arguments**

У	The responses for regmixEM.mixed.
X	The predictors for the random effects in regmixEM.mixed.
W	The predictors for the (optional) fixed effects in regmixEM.mixed.
arb.R	If FALSE, then a test for different variance-covariance matrices for the random effects mixture is performed.
arb.sigma	If FALSE, then a test for different variance terms between the response trajectories is performed.
lambda	A vector of mixing proportions (under the null hypothesis) with same purpose as outlined in ${\tt regmixEM.mixed}$ .
mu	A matrix of the means (under the null hypothesis) with same purpose as outlined in ${\tt regmixEM.mixed.}$
sigma	A vector of standard deviations (under the null hypothesis) with same purpose as outlined in ${\tt regmixEM.mixed}$ .
R	A list of covariance matrices (under the null hypothesis) with same purpose as outlined in ${\tt regmixEM.mixed}$ .
alpha	An optional vector of fixed effects regression coefficients (under the null hypothesis) with same purpose as outlined in regmixEM.mixed.
	Additional arguments passed to regmixEM.mixed.

## Value

test.equality.mixed returns a list with the following items:

chi.sq The chi-squared test statistic.

df The degrees of freedom for the chi-squared test statistic.

p.value The p-value corresponding to this likelihood ratio test.

# See Also

```
test.equality
```

# **Examples**

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```
epsilon = 1e-1, verb = TRUE,
maxit = 50,
addintercept.random = FALSE)
```

out

tonedata

Tone perception data

# Description

The tone perception data stem from an experiment of Cohen (1980) and have been analyzed in de Veaux (1989) and Viele and Tong (2002). The dataset and this documentation file were copied from the fpc package by Christian Hennig. A pure fundamental tone was played to a trained musician. Electronically generated overtones were added, determined by a stretching ratio of stretchratio. stretchratio=2.0 corresponds to the harmonic pattern usually heard in traditional definite pitched instruments. The musician was asked to tune an adjustable tone to the octave above the fundamental tone. tuned gives the ratio of the adjusted tone to the fundamental, i.e. tuned=2.0 would be the correct tuning for all stretchratio-values. The data analyzed here belong to 150 trials with the same musician. In the original study, there were four further musicians.

# Usage

data(tonedata)

## Format

A data frame with 2 variables, stretchratio and tuned, and 150 cases.

# Author(s)

Christian Hennig

# Source

Original source: Cohen, E. A. (1980), *Inharmonic tone perception*. Unpublished Ph.D. dissertation, Stanford University

R source: Hennig, Christian (2010), fpc: Flexible procedures for clustering, R package version 2.0-2. http://CRAN.R-project.org/package=fpc

# References

de Veaux, R. D. (1989), Mixtures of Linear Regressions, *Computational Statistics and Data Analysis* 8, 227-245.

Viele, K. and Tong, B. (2002), Modeling with Mixtures of Linear Regressions, *Statistics and Computing* 12, 315-330.

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Waterdata

Water-Level Task Data Set

#### Description

This data set arises from the water-level task proposed by the Swiss psychologist Jean Piaget to assess children's understanding of the physical world. This involves presenting a child with a rectangular vessel with a cap, affixed to a wall, that can be tilted (like the minute hand of a clock) to point in any direction. A separate disk with a water line indicated on it, which can similarly be spun so that the water line may assume any desired angle with the horizontal, is positioned so that by spinning this disk, the child subject may make the hypothetical surface of water inside the vessel assume any desired orientation. For each of eight different orientations of the vessel, corresponding to the clock angles at 1:00, 2:00, 4:00, 5:00, 7:00, 8:00, 10:00, and 11:00, the child subject is asked to position the water level as it would appear in reality if water were in the vessel. The measurement is the acute angle with the horizontal, in degrees, assumed by the water line after it is positioned by the child. A sign is attached to the measurement to indicate whether the line slopes up (positive) or down (negative) from left to right. Thus, each child has 8 repeated measurements, one for each vessel angle, and the range of possible values are from -90 to 90.

The setup of the experiment, along with a photograph of the testing apparatus, is given by Thomas and Jamison (1975). A more detailed analysis using a subset of 405 of the original 579 subjects is given by Thomas and Lohaus (1993); further analyses using the functions in mixtools are given by Benaglia et al (2008) and Levine et al (2011), among others.

There are two versions of the dataset included in mixtools. The full dataset, called WaterdataFull, has 579 individuals. The dataset called Waterdata is a subset of 405 individuals, comprising all children aged 11 years or more and omitting any individuals with any observations equal to 100, which in this context indicates a missing value (since all of the degree measurements should be in the range from -90 to +90, 100 is not a possible value).

## Usage

Waterdata

#### **Format**

These data frames consist of 405 or 579 rows, one row for each child. There are ten columns: The age (in years) and sex (where 1=male and 0=female) are given for each individual along with the degree of deviation from the horizontal for 8 specified clock-hour orientations (11, 4, 2, 7, 10, 5, 1, and 8 o'clock, in order).

#### Source

Benaglia, T., Chauveau, D., and Hunter, D.R. (2009), An EM-Like Algorithm for Semi- and Non-Parametric Estimation in Multivariate Mixtures, *Journal of Computational and Graphical Statistics*, 18: 505-526.

Levine, M., Hunter, D.R., and Chauveau, D. (2011), Maximum Smoothed Likelihood for Multivariate Mixtures, *Biometrika*, 98(2): 403-416.

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Thomas, H. and Jamison, W. (1975), On the Acquisition of Understanding that Still Water is Horizontal, *Merrill-Palmer Quarterly of Behavior and Development*, 21(1): 31-44.

Thomas, H. and Lohaus, A. (1993), *Modeling Growth and Individual Differences in Spatial Tasks*, University of Chicago Press, Chicago, available on JSTOR.

wkde

Weighted Univariate (Normal) Kernel Density Estimate

# Description

Evaluates a weighted kernel density estimate, using a Gaussian kernel, at a specified vector of points.

# Usage

```
wkde(x, u=x, w=rep(1, length(x)), bw=bw.nrd0(as.vector(x)), sym=FALSE)
```

# **Arguments**

	Data

u Points at which density is to be estimated

w Weights (same length as x)

bw Bandwidth

sym Logical: Symmetrize about zero?

# Value

A vector of the same length as u

## References

- Benaglia, T., Chauveau, D., and Hunter, D. R. (2009), An EM-like algorithm for semi- and non-parametric estimation in multivariate mixtures, Journal of Computational and Graphical Statistics, 18, 505-526.
- Benaglia, T., Chauveau, D., Hunter, D. R., and Young, D. (2009), mixtools: An R package for analyzing finite mixture models. Journal of Statistical Software, 32(6):1-29.

# See Also

```
npEM, ise.npEM
```

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## **Examples**

```
# Mixture with mv gaussian model
set.seed(100)
m \leftarrow 2 \# no. of components
r <- 3 \# no. of repeated measures (coordinates)
lambda <- c(0.4, 0.6)
mu \leftarrow matrix(c(0, 0, 0, 4, 4, 6), m, r, byrow=TRUE) # means
sigma <- matrix(rep(1, 6), m, r, byrow=TRUE) # stdevs</pre>
centers <- matrix(c(0, 0, 0, 4, 4, 4), 2, 3, byrow=TRUE) # initial centers for est
blockid = c(1,1,2) # block structure of coordinates
n = 100
x <- rmvnormmix(n, lambda, mu, sigma) # simulated data
a <- npEM(x, centers, blockid, eps=1e-8, verb=FALSE)
par(mfrow=c(2,2))
u \leftarrow seq(min(x), max(x), len=200)
for(j in 1:2) {
  for(b in 1:2) {
    xx <- as.vector(x[,a$blockid==b])</pre>
    wts <- rep(a$post[,j], length.out=length(xx))</pre>
    bw <- a$bandwidth
    title <- paste("j =", j, "and b =", b)
    plot(u, wkde(xx, u, wts, bw), type="l", main=title)
  }
}
```

wquantile

Weighted quantiles

# Description

Functions to compute weighted quantiles and the weighted interquartile range.

## **Usage**

#### **Arguments**

wt	Vector of weights	
X	Vector of data, same length as wt	
probs	Numeric vector of probabilities with values in [0,1].	

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```
already.sorted If FALSE, sort wt and x in increasing order of x. If TRUE, it is assumed that wt and x are already sorted.

already.normalized
```

If FALSE, normalize wt by diving each entry by the sum of all entries. If TRUE, it is assumed that sum(wt)==1

## **Details**

wquantile uses the findInterval function. wIQR calls the wquantile function.

#### Value

Returns the sample quantiles or interquartile range of a discrete distribution with support points x and corresponding probability masses wt

## See Also

npEM

# **Examples**

```
IQR(1:10) wIQR(x=1:10) # Note: Different algorithm than IQR function wIQR(1:10,1:10) # Weighted quartiles are now 4 and 8
```

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