# Package 'flexmix'

January 27, 2015

Type Package
Title Flexible Mixture Modeling
<b>Version</b> 2.3-13
Description FlexMix implements a general framework for finite mixtures of regression models using the EM algorithm.  FlexMix provides the E-step and all data handling, while the M-step can be supplied by the user to easily define new models. Existing drivers implement mixtures of standard linear models, generalized linear models and model-based clustering.
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Author Bettina Gruen [aut, cre], Friedrich Leisch [aut], Deepayan Sarkar [ctb], Frederic Mortier [ctb], Nicolas Picard [ctb]
Maintainer Bettina Gruen <bettina.gruen@jku.at></bettina.gruen@jku.at>
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# Description

Compute the Akaike Information Criterion.

#### Methods

```
object = flexmix: Compute the AIC of a flexmix object
```

**object = stepFlexmix:** Compute the AIC of all models contained in the stepFlexmix object.

betablocker

Clinical Trial of Beta-Blockers

# Description

22-centre clinical trial of beta-blockers for reducing mortality after myocardial infarction.

# Usage

```
data("betablocker")
```

## **Format**

A data frame with 44 observations on the following 4 variables.

**Deaths** Number of deaths.

Total Total number of patients.

Center Number of clinical centre.

**Treatment** A factor with levels Control and Treated.

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#### **Source**

G. McLachlan and D. Peel. *Finite Mixture Models*, 2000. John Wiley and Sons Inc. http://www.maths.uq.edu.au/~gjm/DATA/mmdata.html

## References

M. Aitkin. Meta-analysis by random effect modelling in generalized linear models. *Statistics in Medicine*, **18**, 2343–2351, 1999.

S. Yusuf, R. Peto, J. Lewis, R. Collins and P. Sleight. Beta blockade during and after myocardial infarction: an overview of the randomized trials. *Progress in Cardiovascular Diseases*, **27**, 335–371, 1985.

## **Examples**

BIC-methods

Methods for Function BIC

# Description

Compute the Bayesian Information Criterion.

#### Methods

```
object = flexmix: Compute the BIC of a flexmix object
object = stepFlexmix: Compute the BIC of all models contained in the stepFlexmix object.
```

bioChemists

Articles by Graduate Students in Biochemistry Ph.D. Programs

# Description

A sample of 915 biochemistry graduate students.

#### Usage

```
data("bioChemists")
```

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#### **Format**

```
art count of articles produced during last 3 years of Ph.D.
fem factor indicating gender of student, with levels Men and Women
mar factor indicating marital status of student, with levels Single and Married
kid5 number of children aged 5 or younger
phd prestige of Ph.D. department
ment count of articles produced by Ph.D. mentor during last 3 years
```

#### **Details**

This data set is taken from package **pscl** provided by Simon Jackman.

#### **Source**

```
found in Stata format at http://www.indiana.edu/~jslsoc/stata/socdata/couart2.dta
```

#### References

Long, J. Scott. The origins of sex difference in science. Social Forces, 68, 1297-1315, 1990.

Long, J. Scott. *Regression Models for Categorical and Limited Dependent Variables*, 1997. Thousand Oaks, California: Sage.

boot

Bootstrap a flexmix Object

## **Description**

Given a flexmix object perform parametric or empirical bootstrap.

## Usage

```
boot(object, ...)
## S4 method for signature 'flexmix'
boot(object, R, sim = c("ordinary", "empirical", "parametric"),
    initialize_solution = FALSE, keep_weights = FALSE,
    keep_groups = TRUE, verbose = 0, control,
    k, model = FALSE, ...)
LR_test(object, ...)
## S4 method for signature 'flexmix'
LR_test(object, R, alternative = c("greater", "less"), control, ...)
```

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#### **Arguments**

object A fitted finite mixture model of class flexmix.

R The number of bootstrap replicates.

sim A character string indicating the type of simulation required. Possible values are

"ordinary" (the default), "parametric", or "empirical".

initialize\_solution

A logical. If TRUE the EM algorithm is initialized in the given solution.

keep\_weights A logical. If TRUE the weights are kept.

keep\_groups A logical. If TRUE the groups are kept.

verbose If a positive integer, then progress information is reported every verbose itera-

tions. If 0, no output is generated during the bootstrap replications.

control Object of class FLXcontrol or a named list. If missing the control of the fitted

object is taken.

k Vector of integers specifying for which number of components finite mixtures

are fitted to the bootstrap samples. If missing the number of components of the

fitted object are taken.

alternative A character string specifying the alternative hypothesis, must be either "greater"

(default) or "less" indicating if the alternative hypothesis is that the mixture has

one more component or one less.

model A logical. If TRUE the model and the weights slot for each sample are stored and

returned.

... Further arguments to be passed to or from methods.

#### Value

boot returns an object of class FLXboot which contains the fitted parameters, the fitted priors, the log likelihoods, the number of components of the fitted mixtures and the information if the EM algorithm has converged.

LR\_test returns an object of class htest containing the number of valid bootstrap replicates, the p-value, the - twice log likelihood ratio test statistics for the original data and the bootstrap replicates.

## Author(s)

Bettina Gruen

# Examples

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BregFix

Artificial Example for Binomial Regression

# Description

A simple artificial regression example data set with 3 latent classes, one independent variable x and a concomitant variable w.

## Usage

```
data("BregFix")
```

#### **Format**

A data frame with 200 observations on the following 5 variables.

```
yes number of successes
no number of failures
x independent variable
w concomitant variable, a factor with levels 0 1
class latent class memberships
```

## **Examples**

candy

Candy Packs Purchased

## **Description**

The data is from a new product and concept test where the number of individual packs of hard candy purchased within the past 7 days is recorded.

#### Usage

```
data("candy")
```

8 dmft

#### **Format**

A data frame with 21 observations on the following 2 variables.

Packages a numeric vector

Freq a numeric vector

#### Source

D. Boehning, E. Dietz and P. Schlattmann. Recent Developments in Computer-Assisted Analysis of Mixtures. Biometrics 54(2), 525–536, 1998.

#### References

- J. Magidson and J. K. Vermunt. Latent Class Models. In D. W. Kaplan (ed.), The Sage Handbook of Quantitative Methodology for the Social Sciences, 175–198, 2004. Thousand Oakes: Sage Publications.
- D. Boehning, E. Dietz and P. Schlattmann. Recent Developments in Computer-Assisted Analysis of Mixtures. *Biometrics*, **54**(2), 525–536, 1998.
- W. R. Dillon and A. Kumar. Latent structure and other mixture models in marketing: An integrative survey and overview. In R. P. Bagozzi (ed.), Advanced methods of marketing research, 352–388, 1994. Cambridge, UK: Blackwell.

dmft

Dental Data

## **Description**

Count data from a dental epidemiological study for evaluation of various programs for reducing caries collected among school children from an urban area of Belo Horizonte (Brazil).

#### **Usage**

data("dmft")

#### **Format**

A data frame with 797 observations on the following 5 variables.

**End** Number of decayed, missing or filled teeth at the end of the study.

**Begin** Number of decayed, missing or filled teeth at the beginning of the study.

Gender A factor with levels male and female.

Ethnic A factor with levels brown, white and black.

**Treatment** A factor with levels control, educ, enrich, rinse, hygiene and all.

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#### **Details**

The aim of the caries prevention study was to compare four methods to prevent dental caries. Interventions were carried out according to the following scheme:

```
control Control group
educ Oral health education
enrich Enrichment of the school diet with rice bran
rinse Mouthwash with 0.2% sodium floride (NaF) solution
hygiene Oral hygiene
all All four methods together
```

#### Source

D. Boehning, E. Dietz, P. Schlattmann, L. Mendonca and U. Kirchner. The zero-inflated Poisson model and the decayed, missing and filled teeth index in dental epidemiology. *Journal of the Royal Statistical Society A*, **162**(2), 195–209, 1999.

## **Examples**

EIC

Entropic Measure Information Criterion

#### **Description**

Compute the Entropic measure Information criterion for model selection.

## Usage

```
## S4 method for signature 'flexmix'
EIC(object, ...)
## S4 method for signature 'stepFlexmix'
EIC(object, ...)
```

## **Arguments**

object see Methods section below
... Some methods for this generic function may take additional, optional arguments.
At present none do.

## Value

Returns a numeric vector with the corresponding EIC value(s).

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#### Methods

```
object = "flexmix": Compute the EIC of a flexmix object.
object = "stepFlexmix": Compute the EIC of all models contained in the stepFlexmix object.
```

#### Author(s)

Bettina Gruen

#### References

V. Ramaswamy, W. S. DeSarbo, D. J. Reibstein, and W. T. Robinson. An empirical pooling approach for estimating marketing mix elasticities with PIMS data. *Marketing Science*, **12**(1), 103–124, 1993.

#### **Examples**

```
data("NPreg", package = "flexmix")
ex1 <- flexmix(yn \sim x + I(x^2), data = NPreg, k = 2)
EIC(ex1)
```

ExLinear

Artificial Data from a Generalized Linear Regression Mixture

# Description

Generate random data mixed from k generalized linear regressions (GLMs).

## Usage

#### **Arguments**

beta	A matrix of regression coefficients. Each row corresponds to a variable, each column to a mixture component. The first row is used as intercept.
n	Integer, the number of observations per component.
xdist	Character, name of a random number function for the explanatory variables.
xdist.args	List, arguments for the random number functions.
family	A character string naming a GLM family. Only "gaussian" and "poisson" are implemented at the moment.
sd	Numeric, the error standard deviation for each component for Gaussian responses.
	Used as default for xdist.args if that is not specified.

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#### **Details**

First, arguments n (and sd for Gaussian response) are recycled to the number of mixture components ncol(beta), and arguments xdist and xdist.args are recycled to the number of explanatory variables nrow(beta)-1. Then a design matrix is created for each mixture component by drawing random numbers from xdist. For each component, the design matrix is multiplied by the regression coefficients to form the linear predictor. For Gaussian responses the identity link is used, for Poisson responses the log link.

The true cluster memberships are returned as attribute "clusters".

#### **Examples**

```
## simple example in 2d
beta <- matrix(c(1, 2, 3, -1), ncol = 2)
sigma < -c(.5, 1)
df1 \leftarrow ExLinear(beta, 100, sd = sigma, min = -1, max = 2)
plot(y~x1, df1, col = attr(df1, "clusters"))
## add a second explanatory variable with exponential distribution
beta2 <- rbind(beta, c(-2, 2))
df2 \leftarrow ExLinear(beta2, 100, sd = c(.5, 1),
                  xdist = c("runif", "rexp"),
                  xdist.args = list(list(min = -1, max = 2),
                                     list(rate = 3)))
summary(df2)
opar = par("mfrow")
par(mfrow = 1:2)
hist(df2$x1)
hist(df2$x2)
par(opar)
f1 \leftarrow flexmix(y \sim ., data = df2, k = 2)
## sort components on Intercept
f1 <- relabel(f1, "model", "Intercept")</pre>
## the parameters should be close to the true beta and sigma
round(parameters(f1), 3)
rbind(beta2, sigma)
### A simple Poisson GLM
df3 <- ExLinear(beta/2, 100, min = -1, max = 2, family = "poisson")
plot(y \sim x1, df3, col = attr(df3, "clusters"))
f3 \leftarrow flexmix(y \sim ., data = df3, k = 2,
              model = FLXMRglm(family = "poisson"))
round(parameters(relabel(f3, "model", "Intercept")), 3)
beta/2
```

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ExNclus

Artificial Example with 4 Gaussians

## **Description**

A simple artificial example for normal clustering with 4 latent classes, all of them having a Gaussian distribution. See the function definition for true means and covariances.

## Usage

```
ExNclus(n)
data("Nclus")
```

## **Arguments**

n

Number of observations in the two small latent classes.

#### **Details**

The Nclus data set can be re-created by ExNclus(100) using set.seed(2602), it has been saved as a data set for simplicity of examples only.

## **Examples**

```
data("Nclus", package = "flexmix")
require("MASS")
eqscplot(Nclus, col = rep(1:4, c(100, 100, 150, 200)))
```

ExNPreg

Artificial Example for Normal, Poisson and Binomial Regression

# Description

A simple artificial regression example with 2 latent classes, one independent variable (uniform on [0, 10]), and three dependent variables with Gaussian, Poisson and Binomial distribution, respectively.

#### Usage

```
ExNPreg(n)
data("NPreg")
```

#### **Arguments**

n

Number of observations per latent class.

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## **Details**

The NPreg data frame can be re-created by ExNPreg(100) using set.seed(2602), it has been saved as a data set for simplicity of examples only.

#### **Examples**

```
data("NPreg", package = "flexmix")
plot(yn ~ x, data = NPreg, col = class)
plot(yp ~ x, data = NPreg, col = class)
plot(yb ~ x, data = NPreg, col = class)
```

fabricfault

Fabric Faults

## **Description**

Number of faults in rolls of a textile fabric.

#### Usage

```
data("fabricfault")
```

#### **Format**

A data frame with 32 observations on the following 2 variables.

Length Length of role (m).

Faults Number of faults.

#### **Source**

G. McLachlan and D. Peel. *Finite Mixture Models*, 2000, John Wiley and Sons Inc. http://www.maths.uq.edu.au/~gjm/DATA/mmdata.html

#### References

A. F. Bissell. A Negative Binomial Model with Varying Element Sizes *Biometrika*, **59**, 435–441, 1972.

M. Aitkin. A general maximum likelihood analysis of overdispersion in generalized linear models. *Statistics and Computing*, **6**, 251–262, 1996.

# Examples

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fitted-methods

Extract Model Fitted Values

## **Description**

Extract fitted values for each component from a flexmix object.

#### Usage

```
## S4 method for signature 'flexmix'
fitted(object, drop = TRUE, aggregate = FALSE, ...)
```

# Arguments

object an object of class "flexmix" or "FLXR"

drop logical, if TRUE then the function tries to simplify the return object by combining

lists of length 1 into matrices.

aggregate logical, if TRUE then the fitted values for each model aggregated over the com-

ponents are returned.

... currently not used

## Author(s)

Friedrich Leisch and Bettina Gruen

## **Examples**

```
data("NPreg", package = "flexmix")
ex1 <- flexmix(yn ~ x + I(x^2), data = NPreg, k = 2)
matplot(NPreg$x, fitted(ex1), pch = 16, type = "p")
points(NPreg$x, NPreg$yn)</pre>
```

flexmix

Flexible Mixture Modeling

## **Description**

FlexMix implements a general framework for finite mixtures of regression models. Parameter estimation is performed using the EM algorithm: the E-step is implemented by flexmix, while the user can specify the M-step.

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#### Usage

#### **Arguments**

formula A symbolic description of the model to be fit. The general form is y~x | g where

y is the response, x the set of predictors and g an optional grouping factor for

repeated measurements.

data An optional data frame containing the variables in the model.

k Number of clusters (not needed if cluster is specified).

cluster Either a matrix with k columns of initial cluster membership probabilities for

each observation; or a factor or integer vector with the initial cluster assignments of observations at the start of the EM algorithm. Default is random assignment

into k clusters.

weights An optional vector of replication weights to be used in the fitting process. Should

be NULL, an integer vector or a formula.

model Object of class FLXM or list of FLXM objects. Default is the object returned by

calling FLXMRglm().

concomitant Object of class FLXP. Default is the object returned by calling FLXPconstant.

control Object of class FLXcontrol or a named list.

object Object of class flexmix.

eps Probabilities below this threshold are treated as zero in the summary method.

... Currently not used.

#### **Details**

FlexMix models are described by objects of class FLXM, which in turn are created by driver functions like FLXMRglm or FLXMCmvnorm. Multivariate responses with independent components can be specified using a list of FLXM objects.

The summary method lists for each component the prior probability, the number of observations assigned to the corresponding cluster, the number of observations with a posterior probability larger than eps and the ratio of the latter two numbers (which indicates how separated the cluster is from the others).

## Value

Returns an object of class flexmix.

## Author(s)

Friedrich Leisch and Bettina Gruen

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#### References

Friedrich Leisch. FlexMix: A general framework for finite mixture models and latent class regression in R. *Journal of Statistical Software*, **11**(8), 2004. http://www.jstatsoft.org/v11/i08/

Bettina Gruen and Friedrich Leisch. Fitting finite mixtures of generalized linear regressions in R. Computational Statistics & Data Analysis, 51(11), 5247-5252, 2007. doi:10.1016/j.csda.2006.08.014

Bettina Gruen and Friedrich Leisch. FlexMix Version 2: Finite mixtures with concomitant variables and varying and constant parameters Journal of Statistical Software, 28(4), 1-35, 2008. URL http://www.jstatsoft.org/v28/i04/

#### See Also

plot-methods

#### **Examples**

```
data("NPreg", package = "flexmix")
## mixture of two linear regression models. Note that control parameters
## can be specified as named list and abbreviated if unique.
ex1 <- flexmix(yn \sim x + I(x^2), data = NPreg, k = 2,
                control = list(verb = 5, iter = 100))
ex1
summary(ex1)
plot(ex1)
## now we fit a model with one Gaussian response and one Poisson
## response. Note that the formulas inside the call to FLXMRglm are
## relative to the overall model formula.
ex2 \leftarrow flexmix(yn \sim x, data = NPreg, k = 2,
                \label{eq:model} \begin{split} \text{model = list(FLXMRglm(yn $^{\sim}$ . + I(x^2)),} \\ \text{FLXMRglm(yp $^{\sim}$ ., family = "poisson")))} \end{split}
plot(ex2)
ex2
table(ex2@cluster, NPreg$class)
## for Gaussian responses we get coefficients and standard deviation
parameters(ex2, component = 1, model = 1)
## for Poisson response we get only coefficients
parameters(ex2, component = 1, model = 2)
## fitting a model only to the Poisson response is of course
## done like this
ex3 <- flexmix(yp \sim x, data = NPreg, k = 2,
                model = FLXMRglm(family = "poisson"))
## if observations are grouped, i.e., we have several observations per
## individual, fitting is usually much faster:
```

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flexmix-class

Class "flexmix"

## **Description**

A fitted flexmix model.

#### Slots

model: List of FLXM objects. prior: Numeric vector with prior probabilities of clusters. posterior: Named list with elements scaled and unscaled, both matrices with one row per observation and one column per cluster. iter: Number of EM iterations. k: Number of clusters after EM. k0: Number of clusters at start of EM. cluster: Cluster assignments of observations. size: Cluster sizes. logLik: Log-likelihood at EM convergence. df: Total number of parameters of the model. components: List describing the fitted components using FLXcomponent objects. formula: Object of class "formula". control: Object of class "FLXcontrol". call: The function call used to create the object. group: Object of class "factor". converged: Logical, TRUE if EM algorithm converged. concomitant: Object of class "FLXP"... weights: Optional weights of the observations.

18 FLXcomponent-class

## **Extends**

```
Class FLXdist, directly.
```

# **Accessor Functions**

The following functions should be used for accessing the corresponding slots:

```
{\tt cluster:} \ \ {\tt Cluster} \ assignments \ of \ observations.
```

posterior: A matrix of posterior probabilities for each observation.

# Author(s)

Friedrich Leisch and Bettina Gruen

FLXcomponent-class

Class "FLXcomponent"

# Description

A fitted component of a flexmix model.

## **Objects from the Class**

Objects can be created by calls of the form new("FLXcomponent", ...).

## **Slots**

```
df: Number of parameters used by the component.
```

logLik: Function computing the log-likelihood of observations.

```
parameters: List with model parameters.
```

predict: Function predicting response for new data.

# Author(s)

Friedrich Leisch and Bettina Gruen

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FLXcontrol-class

Class "FLXcontrol"

## Description

Hyperparameters for the EM algorithm.

## **Objects from the Class**

Objects can be created by calls of the form new("FLXcontrol", ...). In addition, named lists can be coerced to FLXcontrol objects, names are completed if unique (see examples).

#### **Slots**

iter.max: Maximum number of iterations.

minprior: Minimum prior probability of clusters, components falling below this threshold are removed during the iteration.

tolerance: The EM algorithm is stopped when the (relative) change of log-likelihood is smaller than tolerance.

verbose: If a positive integer, then the log-likelihood is reported every verbose iterations. If 0, no output is generated during model fitting.

```
classify: Character string, one of "auto", "weighted", "hard" (or "CEM"), "random" or ("SEM").
```

nrep: Reports the number of random initializations used in stepFlexmix() to determine the mixture.

Run new("FLXcontrol") to see the default settings of all slots.

## Author(s)

Friedrich Leisch and Bettina Gruen

## **Examples**

```
## have a look at the defaults
new("FLXcontrol")

## corce a list
mycont <- list(iter = 200, tol = 0.001, class = "r")
as(mycont, "FLXcontrol")</pre>
```

20 FLXdist

# Description

Constructs objects of class FLXdist which represent unfitted finite mixture models.

# Usage

# Arguments

formula	A symbolic description of the model to be fit. The general form is $\sim x \mid g$ where x is the set of predictors and g an optional grouping factor for repeated measurements.
k	Integer specifying the number of cluster or a numeric vector of length equal to the length of components, specifying the prior probabilities of clusters.
mode1	Object of class FLXM or a list of FLXM objects. Default is the object returned by calling FLXMRg1m().
components	A list of length equal to the number of components containing a list of length equal to the number of models which again contains a list of named elements for defining the parameters of the component-specific model.
concomitant	Object of class FLXconcomitant specifying the model for concomitant variables.

# Value

Returns an object of class FLXdist.

# Author(s)

Bettina Gruen

## See Also

FLXdist-class

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# Description

Objects of class FLXdist represent unfitted finite mixture models.

# Usage

# Arguments

object	An object of class "FLXdist".
component	Number of component(s), if NULL all components are returned.
model	Number of model(s), if NULL all models are returned.
which	Specifies if the parameters of the component specific model or the concomitant variable model are returned.
simplify	Logical, if TRUE the returned values are simplified to a vector or matrix if possible. $ \\$
drop	Logical, if TRUE the function tries to simplify the return object by omitting lists of length one. $ \\$
newdata	Dataframe containing new data.
aggregate	Logical, if TRUE then the predicted values for each model aggregated over the components are returned. $$
	Passed to the method of the model class.

## **Slots**

model List of FLXM objects.

prior Numeric vector with prior probabilities of clusters.

components List describing the components using FLXcomponent objects.

concomitant: Object of class "FLXP".

formula Object of class "formula".

call The function call used to create the object.

k Number of clusters.

22 FLXfit

#### **Accessor Functions**

The following functions should be used for accessing the corresponding slots:

parameters: The parameters for each model and component, return value depends on the model.

prior: Numeric vector of prior class probabilities/component weights

#### Author(s)

Friedrich Leisch and Bettina Gruen

#### See Also

FLXdist

FLXfit

Fitter Function for FlexMix Models

## **Description**

This is the basic computing engine called by flexmix, it should usually not be used directly.

## Usage

## **Arguments**

model List of FLXM objects.
concomitant Object of class FLXP.

control Object of class FLXcontrol.

weights A numeric vector of weights to be used in the fitting process.

postunscaled Initial a-posteriori probabilities of the observations at the start of the EM algo-

rithm.

groups List with components group which is a factor with optional grouping of obser-

vations and groupfirst which is a logical vector for the first observation of

each group.

## Value

Returns an object of class flexmix.

## Author(s)

Friedrich Leisch and Bettina Gruen

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## See Also

flexmix, flexmix-class

FLXM-class

Class "FLXM"

#### **Description**

FlexMix model specification.

## **Objects from the Class**

Objects can be created by calls of the form new("FLXM", ...), typically inside driver functions like FLXMRglm or FLXMCmvnorm.

#### **Slots**

fit: Function returning an FLXcomponent object.

defineComponent: Expression to determine the FLXcomponent object given the parameters.

weighted: Logical indicating whether fit can do weighted likelihood maximization.

name: Character string used in print methods.

formula: Formula describing the model.

fullformula: Resulting formula from updating the model formula with the formula specified in the call to flexmix.

x: Model matrix.

y: Model response.

terms, xlevels, contrasts: Additional information for model matrix.

preproc.x: Function for preprocessing matrix x before the EM algorithm starts, by default the identity function.

preproc.y: Function for preprocessing matrix y before the EM algorithm starts, by default the identity function.

## Author(s)

Friedrich Leisch and Bettina Gruen

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FLXMCfactanal	Driver for Mixtures of Factor Analyzers	

# Description

This driver for flexmix implements estimation of mixtures of factor analyzers using ML estimation of factor analysis implemented in factanal in each M-step.

# Usage

```
FLXMCfactanal(formula = . ~ ., factors = 1, ...)
```

# Arguments

formula	A formula which is interpreted relative to the formula specified in the call to flexmix using update.formula. Only the left-hand side (response) of the formula is used. Default is to use the original flexmix model formula.
factors	Integer specifying the number of factors in each component.
	Passed to factanal

## Value

FLXMCfactanal returns an object of class FLXM.

## Warning

This does not implement the AECM framework presented in McLachlan and Peel (2000, p.245), but uses the available functionality in R for ML estimation of factor analyzers. The implementation therefore is only experimental and has not been well tested.

Please note that in general a good initialization is crucial for the EM algorithm to converge to a suitable solution for this model class.

## Author(s)

Bettina Gruen

# References

G. McLachlan and D. Peel. Finite Mixture Models, 2000. John Wiley and Sons Inc.

#### See Also

flexmix

FLXMCmvbinary 25

#### **Examples**

```
## Reproduce (partly) Table 8.1. p.255 (McLachlan and Peel, 2000)
if (require("gclus")) {
 data("wine", package = "gclus")
 wine_data <- as.matrix(wine[,-1])</pre>
 set.seed(123)
 wine_fl_diag <- initFlexmix(wine_data ~ 1, k = 3, nrep = 10,</pre>
                               model = FLXMCmvnorm(diagonal = TRUE))
 wine_fl_fact <- lapply(1:4, function(q) flexmix(wine_data ~ 1, model =</pre>
                           FLXMCfactanal(factors = q, nstart = 3),
                           cluster = posterior(wine_fl_diag)))
 sapply(wine_fl_fact, logLik)
 ## FULL
 set.seed(123)
 wine_full <- initFlexmix(wine_data ~ 1, k = 3, nrep = 10,</pre>
                            model = FLXMCmvnorm(diagonal = FALSE))
 logLik(wine_full)
 ## TRUE
 wine_true <- flexmix(wine_data ~ 1, cluster = wine$Class,</pre>
                        model = FLXMCmvnorm(diagonal = FALSE))
 logLik(wine_true)
}
```

FLXMCmvbinary

FlexMix Binary Clustering Driver

## **Description**

This is a model driver for flexmix implementing model-based clustering of binary data.

#### Usage

```
FLXMCmvbinary(formula = . ~ ., truncated = FALSE)
```

#### **Arguments**

formula A formula which is interpreted relative to the formula specified in the call to

flexmix using update. formula. Only the left-hand side (response) of the for-

mula is used. Default is to use the original flexmix model formula.

truncated logical, if TRUE the observations for the pattern with only zeros are missing and

the truncated likelihood is optimized using an EM-algorithm.

# Details

This model driver can be used to cluster binary data. The only parameter is the column-wise mean of the data, which equals the probability of observing a 1.

26 FLXMCmvcombi

#### Value

FLXMCmvbinary returns an object of class FLXMC.

## Author(s)

Friedrich Leisch and Bettina Gruen

#### See Also

flexmix

FLXMCmvcombi

FlexMix Binary and Gaussian Clustering Driver

## **Description**

This is a model driver for flexmix implementing model-based clustering of a combination of binary and Gaussian data.

## Usage

```
FLXMCmvcombi(formula = . ~ .)
```

## **Arguments**

formula

A formula which is interpreted relative to the formula specified in the call to flexmix using update.formula. Only the left-hand side (response) of the formula is used. Default is to use the original flexmix model formula.

#### **Details**

This model driver can be used to cluster mixed-mode binary and Gaussian data. It checks which columns of a matrix contain only zero and ones, and does the same as FLXMCmvbinary for them. For the remaining columns of the data matrix independent Gaussian distributions are used (same as FLXMCmvnorm with diagonal = FALSE. The same could be obtained by creating a corresponding list of two models for the respective columns, but FLXMCmvcombi does a better job in reporting parameters.

## Value

FLXMCmvcombi returns an object of class FLXMC.

## Author(s)

Friedrich Leisch

FLXMCmvnorm 27

## See Also

flexmix, FLXMCmvbinary, FLXMCmvnorm

#### **Examples**

```
## create some artificial data
x1 <- cbind(rnorm(300),
             sample(0:1, 300, replace = TRUE, prob = c(0.25, 0.75))
x2 < - cbind(rnorm(300, mean = 2, sd = 0.5),
            sample(0:1, 300, replace = TRUE, prob = c(0.75, 0.25))
x \leftarrow rbind(x1, x2)
## fit the model
f1 <- flexmix(x \sim 1, k = 2, model = FLXMCmvcombi())
## should be similar to the original parameters
parameters(f1)
table(clusters(f1), rep(1:2, c(300,300)))
## a column with noise should not hurt too much
x \leftarrow cbind(x, rnorm(600))
f2 \leftarrow flexmix(x \sim 1, k = 2, model = FLXMCmvcombi())
parameters(f2)
table(clusters(f2), rep(1:2, c(300,300)))
```

**FLXMCmvnorm** 

FlexMix Clustering Demo Driver

#### Description

These are demo drivers for flexmix implementing model-based clustering of Gaussian data.

## Usage

```
FLXMCmvnorm(formula = . ~ ., diagonal = TRUE)
FLXMCnorm1(formula = . ~ .)
```

## **Arguments**

formula A formula which is interpreted relative to the formula specified in the call to flexmix using update. formula. Only the left-hand side (response) of the formula is used. Default is to use the original flexmix model formula.

diagonal If TRUE, then the covariance matrix of the components is restricted to diagonal

matrices.

#### **Details**

This is mostly meant as a demo for FlexMix driver programming, you should also look at package **mclust** for real applications. FLXMCmvnorm clusters multivariate data, FLXMCnorm1 univariate data. In the latter case smart initialization is important, see the example below.

28 FLXMCmvnorm

#### Value

FLXMCmvnorm returns an object of class FLXMC.

#### Author(s)

Friedrich Leisch and Bettina Gruen

#### References

Friedrich Leisch. FlexMix: A general framework for finite mixture models and latent class regression in R. *Journal of Statistical Software*, **11**(8), 2004. http://www.jstatsoft.org/v11/i08/

#### See Also

flexmix

## **Examples**

```
data("Nclus", package = "flexmix")
require("MASS")
eqscplot(Nclus)
## This model is wrong (one component has a non-diagonal cov matrix)
ex1 <- flexmix(Nclus ~ 1, k = 4, model = FLXMCmvnorm())
print(ex1)
plotEll(ex1, Nclus)
## True model, wrong number of components
ex2 <- flexmix(Nclus ~ 1, k = 6, model = FLXMCmvnorm(diagonal = FALSE))
print(ex2)
plotEll(ex2, Nclus)
## Get parameters of first component
parameters(ex2, component = 1)
## Have a look at the posterior probabilies of 10 random observations
ok <- sample(1:nrow(Nclus), 10)</pre>
  <- posterior(ex2)[ok, ]</pre>
## The following two should be the same
max.col(p)
clusters(ex2)[ok]
## Now try the univariate case
plot(density(Nclus[, 1]))
ex3 <- flexmix(Nclus[, 1] ~ 1, cluster = cut(Nclus[, 1], 3),
               model = FLXMCnorm1())
ex3
```

FLXMCmvpois 29

```
parameters(ex3)
```

FLXMCmvpois

FlexMix Poisson Clustering Driver

# Description

This is a model driver for flexmix implementing model-based clustering of Poisson distributed data

# Usage

```
FLXMCmvpois(formula = . ~ .)
```

## **Arguments**

formula

A formula which is interpreted relative to the formula specified in the call to flexmix using update.formula. Only the left-hand side (response) of the formula is used. Default is to use the original flexmix model formula.

## **Details**

This can be used to cluster Poisson distributed data where given the component membership the variables are mutually independent.

## Value

FLXMCmvpois returns an object of class FLXMC.

#### Author(s)

Friedrich Leisch and Bettina Gruen

## See Also

flexmix

30 FLXMRcondlogit

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FlexMix Interface to Conditional Logit Models

## **Description**

Model driver for fitting mixtures of conditional logit models.

## Usage

```
FLXMRcondlogit(formula = . ~ ., strata)
```

# Arguments

formula A formula which is interpreted relative to the formula specified in the call to

flexmix using update.formula. Default is to use the original flexmix model

formula.

strata A formula which is interpreted such that no intercept is fitted and which allows

to determine the variable indicating which observations are from the same stra-

tum.

#### **Details**

The M-step is performed using coxph.fit.

#### Value

Returns an object of class FLXMRcondlogit.

# Warning

To ensure identifiability repeated measurements are necessary. Sufficient conditions are given in Gruen and Leisch (2008).

#### Author(s)

Bettina Gruen

## References

Bettina Gruen and Friedrich Leisch. Identifiability of finite mixtures of multinomial logit models with varying and fixed effects. *Journal of Classification*, **25**, 225–247. 2008.

#### See Also

FLXMRmultinom

FLXMRglm 31

## **Examples**

```
if (require("mlogit")) {
 data("Catsup", package = "mlogit")
 ## To reduce the time needed for the example only a subset is used
 Catsup <- subset(Catsup, id %in% 1:100)</pre>
 Catsup$experiment <- seq_len(nrow(Catsup))</pre>
 vnames <- c("display", "feature", "price")</pre>
 Catsup_long <-
    reshape(Catsup,
            idvar = c("id", "experiment"),
            times = c(paste("heinz", c(41, 32, 28), sep = ""),
              "hunts32"),
            timevar = "brand",
            varying = matrix(colnames(Catsup)[2:13], nrow = 3, byrow = TRUE),
            v.names = vnames,
            direction = "long")
 Catsup_long$selected <- with(Catsup_long, choice == brand)</pre>
 Catsup_long <- Catsup_long[, c("id", "selected", "experiment", vnames, "brand")]</pre>
 Catsup_long$brand <- relevel(factor(Catsup_long$brand), "hunts32")</pre>
 set.seed(0808)
 flx1 <- flexmix(selected ~ display + feature + price + brand | id,
                  model = FLXMRcondlogit(strata = ~ experiment),
                  data = Catsup\_long, k = 1)
}
```

FLXMRg1m

FlexMix Interface to Generalized Linear Models

## **Description**

This is the main driver for FlexMix interfacing the glm family of models.

## Usage

```
FLXMRglm(formula = . ~ .,
         family = c("gaussian", "binomial", "poisson", "Gamma"),
         offset = NULL)
```

## **Arguments**

formula	A formula which is interpreted relative to the formula specified in the call to
	flexmix using update.formula. Default is to use the original flexmix model

formula.

A character string naming a glm family function. family

This can be used to specify an a priori known component to be included in the offset

linear predictor during fitting.

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#### **Details**

See flexmix for examples.

#### Value

Returns an object of class FLXMRglm.

## Author(s)

Friedrich Leisch and Bettina Gruen

#### References

Friedrich Leisch. FlexMix: A general framework for finite mixture models and latent class regression in R. *Journal of Statistical Software*, **11**(8), 2004. http://www.jstatsoft.org/v11/i08/

#### See Also

```
flexmix, glm
```

 ${\sf FLXMRglmfix}$ 

FlexMix Interface to GLMs with Fixed Coefficients

## **Description**

This implements a driver for FlexMix which interfaces the glm family of models and where it is possible to specify fixed (constant) or nested varying coefficients or to ensure that in the Gaussian case the variance estimate is equal for all components.

#### Usage

## **Arguments**

formula	A formula which is interpreted relative to the formula specified in the call to flexmix using update.formula. Default is to use the original flexmix model formula.
fixed	A formula which specifies the additional regressors for the fixed (constant) coefficients.
varFix	A logical indicating if the variance estimate for Gaussian components should be constrained to be equal for all components. It can be also a vector specifying the number of components with equal variance.
nested	An object of class FLXnested or a list specifying the nested structure.

FLXMRglmnet 33

family A character string naming a glm family function.

offset This can be used to specify an a priori known component to be included in the

linear predictor during fitting.

#### Value

Returns an object of class FLXMRglmfix.

#### Author(s)

Friedrich Leisch and Bettina Gruen

#### See Also

FLXMRglm

## **Examples**

FLXMRglmnet

FlexMix Interface for Adaptive Lasso / Elastic Net with GLMs

# Description

This is a driver which allows fitting of mixtures of GLMs where the coefficients are penalized using the (adaptive) lasso or the elastic net by reusing functionality from package **glmnet**.

## Usage

34 FLXMRgImnet

## **Arguments**

formula	A formula which is interpreted relative to the formula specified in the call to flexmix using update.formula. Default is to use the original flexmix model formula.
family	A character string naming a glm family function.
adaptive	A logical indicating if the adaptive lasso should be used. By default equal to $TRUE.$
select	A logical vector indicating which variables in the model matrix should be included in the penalized part. By default equal to TRUE implying that all variables are penalized.
offset	This can be used to specify an <i>a priori</i> known component to be included in the linear predictor during fitting.
	Additional arguments to be passed to cv.glmnet fitter.

#### **Details**

Some care is needed to ensure convergence of the algorithm, which is computationally more challenging than a standard EM. In the proposed method, not only are cluster allocations identified and component parameters estimated as commonly done in mixture models, but there is also variable selection via penalized regression using \$k\$-fold cross-validation to choose the penalty parameter. For the algorithm to converge, it is necessary that the same cross-validation partitioning be used across the EM iterations, i.e., the subsamples for cross-validation must be defined at the beginning This is accomplished using the foldid option as an additional parameter to be passed to cv.glmnet (see glmnet package documentation).

#### Value

Returns an object of class FLXMRg1m.

## Author(s)

Frederic Mortier and Nicolas Picard.

#### References

Frederic Mortier, Dakis-Yaoba Ouedraogo, Florian Claeys, Mahlet G. Tadesse, Guillaume Cornu, Fidele Baya, Fabrice Benedet, Vincent Freycon, Sylvie Gourlet-Fleury and Nicolas Picard. Mixture of inhomogeneous matrix models for species-rich ecosystems. *Environmetrics*, in press. doi:10.1002/env.2320

## See Also

FLXMRg1m

FLXMRImer 35

#### **Examples**

```
set.seed(12)
p <- 10
beta <- matrix(0, nrow = p + 1, ncol = 2)
beta[1,] <- c(-1, 1)
beta[cbind(c(5, 10), c(1, 2))] <- 1
nobs <- 100
X <- matrix(rnorm(nobs * p), nobs, p)</pre>
mu <- cbind(1, X) %*% beta
z <- sample(1:ncol(beta), nobs, replace = TRUE)</pre>
y <- mu[cbind(1:nobs, z)] + rnorm(nobs)</pre>
data <- data.frame(y, X)</pre>
## The maximum number of iterations is reduced to
## avoid a long running time.
fo <- sample(rep(seq(10), length = nrow(data)))</pre>
ex1 <- flexmix(y \sim ., data = data, k = 2, cluster = z,
               model = FLXMRglmnet(foldid = fo),
                control = list(iter.max = 2))
parameters(ex1)
```

FLXMR1mer

FlexMix Interface to Linear Mixed Models

#### **Description**

This is a driver which allows fitting of mixtures of linear models with random effects.

## Usage

## **Arguments**

formula	A formula which is interpreted relative to the formula specified in the call to flexmix using update.formula. Default is to use the original flexmix model formula.
random	A formula for specifying the random effects.
weighted	A logical indicating if the model should be estimated with weighted ML.
control	A list of control parameters. See lmer for details.
eps	Observations with a component-specific posterior smaller than eps are omitted in the M-step for this component.

36 FLXMRImmc

lm.fit	A character string indicating if the coefficients should be fitted using either a linear model or the function smooth.spline
varFix	Named logical vector of length 2 indicating if the variance of the random effects and the residuals are fixed over the components.
	Additional arguments to be passed to smooth.spline.

#### **Details**

FLXMRlmm allows only one random effect. FLXMRlmer allows an arbitrary number of random effects if weighted = FALSE; a certain structure of the model matrix of the random effects has to be given for weighted ML estimation, i.e. where weighted = TRUE.

#### Value

Returns an object of class FLXMRlmer and FLXMRlmm.

# Warning

For FLXMRlmer the weighted ML estimation is only correct if the covariate matrix of the random effects is the same for each observation. By default weighted ML estimation is made and the condition on the covariate matrix of the random effects is checked. If this fails, only estimation with weighted = FALSE is possible which will maximize the classification likelihood.

## Author(s)

Bettina Gruen

## **Examples**

FLXMR1mmc

FlexMix Interface to Linear Mixed Models with Left-Censoring

#### **Description**

This is a driver which allows fitting of mixtures of linear models with random effects and left-censored observations.

FLXMRmgcv 37

## Usage

```
FLXMRlmmc(formula = . ~ ., random, censored, varFix, eps = 10^-6, ...)
```

## **Arguments**

formula	A formula which is interpreted relative to the formula specified in the call to flexmix using update.formula. Default is to use the original flexmix model formula.
random	A formula for specifying the random effects. If missing no random effects are fitted.
varFix	If random effects are specified a named logical vector of length 2 indicating if the variance of the random effects and the residuals are fixed over the components. Otherwise a logical indicating if the variance of the residuals are fixed over the components.
censored	A formula for specifying the censoring variable.
eps	Observations with an a-posteriori probability smaller or equal to eps are omitted in the M-step.
	Additional arguments to be passed to lm.wfit.

## Value

Returns an object of class FLXMRlmmc, FLXMRlmmcfix, FLXMRlmc or FLXMRlmcfix.

# Author(s)

Bettina Gruen

FLXMRmgcv	FlexMix Interface to GAMs	

# Description

This is a driver which allows fitting of mixtures of GAMs.

## Usage

38 FLXMRmgcv

# **Arguments**

formula	A formula which is interpreted relative to the formula specified in the call to flexmix using update.formula. Default is to use the original flexmix model formula.
family	A character string naming a glm family function.
offset	This can be used to specify an <i>a priori</i> known component to be included in the linear predictor during fitting.
control	A list of fit control parameters returned by gam. control.
optimizer	An array specifying the numerical optimization method to use to optimize the smoothing parameter estimation criterion; for more details see gam.
in.out	Optional list for initializing outer iteration; for more details see gam.
eps	Observations with an a-posteriori probability smaller or equal to eps are omitted in the M-step.
	Additional arguments to be pased to the GAM fitter.

## Value

Returns an object of class FLXMRmgcv.

## Author(s)

Bettina Gruen

# See Also

FLXMRg1m

FLXMRmultinom 39

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FlexMix Interface to Multiomial Logit Models

# Description

Model driver for fitting mixtures of multinomial logit models.

## Usage

```
FLXMRmultinom(formula = . ~ ., ...)
```

## **Arguments**

formula A formula which is interpreted relative to the formula specified in the call to

flexmix using update.formula. Default is to use the original flexmix model

formula.

... Additional arguments to be passed to nnet.default.

## **Details**

The M-step is performed using nnet.default.

#### Value

Returns an object of class FLXMRmultinom.

## Warning

To ensure identifiability repeated measurements are necessary. Sufficient conditions are given in Gruen and Leisch (2008).

# Author(s)

Bettina Gruen

## References

Bettina Gruen and Friedrich Leisch. Identifiability of finite mixtures of multinomial logit models with varying and fixed effects. *Journal of Classification*, **25**, 225–247. 2008.

## See Also

FLXMRcondlogit

40 FLXMRrobglm

FLXMRrobglm FlexMix Driver for Robust Estimation of Generalized Linear Model.	S
---	---

## **Description**

This driver adds a noise component to the mixture model which can be used to model background noise in the data. See the Compstat paper Leisch (2008) cited below for details.

## Usage

## **Arguments**

formula	A formula which is interpreted relative to the formula specified in the call to flexmix using update.formula. Default is to use the original flexmix model formula.
family	A character string naming a glm family function.
bgw	Logical, controls whether the parameters of the background component are fixed to multiples of location and scale of the complete data (the default), or estimated by EM with normal weights for the background (bgw = TRUE).
	passed to FLXMRglm

## Value

Returns an object of class FLXMRrobglm.

## Note

The implementation of this model class is currently under development, and some methods like refit are still missing.

## Author(s)

Friedrich Leisch and Bettina Gruen

## References

Friedrich Leisch. Modelling background noise in finite mixtures of generalized linear regression models. In Paula Brito, editor, Compstat 2008–Proceedings in Computational Statistics, 385–396. Physica Verlag, Heidelberg, Germany, 2008.

Preprint available at http://epub.ub.uni-muenchen.de/6332/.

FLXMRziglm 41

## **Examples**

```
## Example from Compstat paper, see paper for detailed explanation:
data("NPreg", package = "flexmix")
DATA <- NPreg[, 1:2]
set.seed(3)
DATA2 <- rbind(DATA, cbind(x = -runif(3), yn = 50 + runif(3)))
## Estimation without (f2) and with (f3) background component
f2 \leftarrow flexmix(yn \sim x + I(x^2), data = DATA2, k = 2)
f3 <- flexmix(yn \sim x + I(x^2), data = DATA2, k = 3,
              model = FLXMRrobglm(),
              control = list(minprior = 0))
## Predict on new data for plots
x < - seq(-5, 15, by = .1)
y2 \leftarrow predict(f2, newdata = data.frame(x = x))
y3 \leftarrow predict(f3, newdata = data.frame(x = x))
## f2 was estimated without background component:
plot(yn \sim x, data = DATA2, pch = clusters(f2), col = clusters(f2))
lines(x, y2$Comp.1, col = 1)
lines(x, y2$Comp.2, col = 2)
## f3 is with background component:
plot(yn \sim x, data = DATA2, pch = 4 - clusters(f3),
     col = 4 - clusters(f3))
lines(x, y3$Comp.2, col = 2)
lines(x, y3$Comp.3, col = 1)
```

FLXMRziglm

FlexMix Interface to Zero Inflated Generalized Linear Models

#### **Description**

This is a driver which allows fitting of zero inflated poisson and binomial models.

## Usage

```
FLXMRziglm(formula = . ~ ., family = c("binomial", "poisson"), ...)
```

# **Arguments**

formula	A formula which is interpreted relative to the formula specified in the call to flexmix using update.formula. Default is to use the original flexmix model formula.
family	A character string naming a glm family function.
	passed to FLXMRglm

42 FLXnested-class

## Value

Returns an object of class FLXMRziglm.

## Note

In fact this only approximates zero inflated models by fixing the coefficient of the intercept at -Inf and the other coefficients at zero for the first component.

## Author(s)

Friedrich Leisch and Bettina Gruen

## **Examples**

FLXnested-class

Class "FLXnested"

## **Description**

Specification of nesting structure for regression coefficients.

# **Objects from the Class**

Objects can be created by calls of the form new("FLXnested", formula, k, ...). In addition, named lists can be coerced to FLXnested objects, names are completed if unique.

## **Slots**

formula: Object of class "list" containing the formula for determining the model matrix for each nested parameter.

k: Object of class "numeric" specifying the number of components in each group.

## Author(s)

Friedrich Leisch and Bettina Gruen

FLXP 43

**FLXP** 

Creates the Concomitant Variable Model

# **Description**

Creator functions for the concomitant variable model. FLXPconstant specifies constant priors and FLXPmultinom multinomial logit models for the priors.

## Usage

```
FLXPconstant()
FLXPmultinom(formula = ~1)
```

## Arguments

formula

A formula for determining the model matrix of the concomitant variables.

## **Details**

FLXPmultinom uses nnet.default from nnet to fit the multinomial logit model.

## Value

Object of class FLXP. FLXPmultinom returns an object of class FLXPmultinom which extends class FLXP directly and is used for method dispatching.

## Author(s)

Friedrich Leisch and Bettina Gruen

FLXP-class

Class "FLXP"

# Description

Concomitant model class.

## **Objects from the Class**

Objects can be created by calls of the form new("FLXP", ...), typically inside driver functions like FLXPconstant or FLXPmultinom.

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## **Slots**

```
name: Character string used in print methods.

formula: Formula describing the model.

x: Model matrix.

fit: Function returning the fitted prior probabilities.

refit: Function returning the fitted concomitant model.

coef: Matrix containing the fitted parameters.

df: Function for determining the number of degrees of freedom used.
```

## Author(s)

Friedrich Leisch and Bettina Gruen

group

Extract Grouping Variable

# Description

Extract grouping variable for all observations.

# Usage

```
## S4 method for signature 'flexmix'
group(object)
## S4 method for signature 'FLXM'
group(object)
## S4 method for signature 'FLXMRglmfix'
group(object)
```

## **Arguments**

object an object of class flexmix.

# Author(s)

Bettina Gruen

Integrated Completed Likelihood Criterion

ICL

# Description

Compute the Integrated Completed Likelihood criterion for model selection.

## Usage

```
## S4 method for signature 'flexmix'
ICL(object, ...)
## S4 method for signature 'stepFlexmix'
ICL(object, ...)
```

## Arguments

object see Methods section below
... Some methods for this generic function may take additional, optional arguments.
At present none do.

#### Value

Returns a numeric vector with the corresponding ICL value(s).

## Methods

```
object = "flexmix": Compute the ICL of a flexmix object.
object = "stepFlexmix": Compute the ICL of all models contained in the stepFlexmix object.
```

# Author(s)

Friedrich Leisch and Bettina Gruen

## References

C. Biernacki, G. Celeux, and G. Govaert. Assessing a mixture model for clustering with the integrated completed likelihood. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 22(7), 719–725, 2000.

```
data("NPreg", package = "flexmix")
ex1 <- flexmix(yn \sim x + I(x^2), data = NPreg, k = 2)
ICL(ex1)
```

46 KLdiv

KLdiv

Kullback-Leibler Divergence

## **Description**

Estimate the Kullback-Leibler divergence of several distributions.

# Usage

```
## S4 method for signature 'matrix'
KLdiv(object, eps = 10^-4, overlap = TRUE,...)
## S4 method for signature 'flexmix'
KLdiv(object, method = c("continuous", "discrete"), ...)
```

# Arguments

object	See Methods section below.
method	The method to be used; "continuous" determines the Kullback-Leibler divergence between the unweighted theoretical component distributions and the unweighted posterior probabilities at the observed points are used by "discrete".
eps	Probabilities below this threshold are replaced by this threshold for numerical stability.
overlap	Logical, do not determine the KL divergence for those pairs where for each point at least one of the densities has a value smaller than eps.
	Passed to the matrix method.

## **Details**

Estimates

$$\int f(x)(\log f(x) - \log g(x))dx$$

for distributions with densities f() and g().

## Value

A matrix of KL divergences where the rows correspond to using the respective distribution as f() in the formula above.

## Methods

**object = "matrix":** Takes as input a matrix of density values with one row per observation and one column per distribution.

**object = "flexmix":** Returns the Kullback-Leibler divergence of the mixture components.

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## Note

The density functions are modified to have equal support. A weight of at least eps is given to each observation point for the modified densities.

## Author(s)

Friedrich Leisch and Bettina Gruen

#### References

S. Kullback and R. A. Leibler. On information and sufficiency. *The Annals of Mathematical Statistics*, **22**(1), 79–86, 1951.

Friedrich Leisch. Exploring the structure of mixture model components. In Jaromir Antoch, editor, Compstat 2004–Proceedings in Computational Statistics, 1405–1412. Physika Verlag, Heidelberg, Germany, 2004. ISBN 3-7908-1554-3.

## **Examples**

Lapply-methods

Methods for Function Lapply

## **Description**

Apply a function to each component of a finite mixture

## Usage

```
## S4 method for signature 'FLXRmstep'
Lapply(object, FUN, model = 1, component = TRUE, ...)
```

48 logLik-methods

## Arguments

object S4 class object.

FUN The function to be applied.

model The model (for a multivariate response) that shall be used.

component Index vector for selecting the components.

... Optional arguments to FUN.

#### Details

FUN is found by a call to match. fun and typically is specified as a function or a symbol (e.g. a back-quoted name) or a character string specifying a function to be searched for from the environment of the call to Lapply.

#### Value

A list of the length equal to the number of components specified is returned, each element of which is the result of applying FUN to the specified component of the refitted mixture model.

#### Methods

**object = FLXRmstep:** Apply a function to each component of a refitted flexmix object using method = "mstep".

#### Author(s)

Friedrich Leisch and Bettina Gruen

# **Examples**

logLik-methods

Methods for Function logLik in Package flexmix

# Description

Evaluate the log-likelihood. This function is defined as an S4 generic in the stats4 package.

#### Methods

**object = flexmix** Evaluate the log-likelihood of an flexmix object

Mehta 49

Mehta Mehta Trial

## **Description**

For a 22-centre trial the number of responses and the total number of patients is reported for the control group and the group receiving a new drug.

## Usage

```
data("Mehta")
```

#### **Format**

A data frame with 44 observations on the following 4 variables.

Response Number of responses.

Total Total number of observations.

**Drug** A factor indicating treatment with levels New and Control.

**Site** A factor indicating the site/centre.

## Source

M. Aitkin. Meta-analysis by random effect modelling in generalized linear models. *Statistics in Medicine*, **18**, 2343–2351, 1999.

#### References

C.R. Mehta, N.R. Patel and P. Senchaudhuri. Importance sampling for estimating exact probabilities in permutational inference. *Journal of the American Statistical Association*, 83, 999–1005, 1988.

50 patent

NregFix

Artificial Example for Normal Regression

## **Description**

A simple artificial regression example with 3 latent classes, two independent variables, one concomitant variable and a dependent variable which follows a Gaussian distribution.

# Usage

```
data("NregFix")
```

#### **Format**

A data frame with 200 observations on the following 5 variables.

- x1 Independent variable: numeric variable.
- x2 Independent variable: a factor with two levels: 0 and 1.
- w Concomitant variable: a factor with two levels: 0 and 1.
- y Dependent variable.
- class Latent class memberships.

## **Examples**

patent

Patents and R&D Spending

## **Description**

Number of patents, R&D spending and sales in millions of dollar for 70 pharmaceutical and biomedical companies in 1976.

#### Usage

```
data("patent")
```

plot-methods 51

## **Format**

A data frame with 70 observations on the following 4 variables.

Company Name of company.

Patents Number of patents.

**RDS** R&D spending per sales.

**lgRD** Logarithmized R&D spendings (in millions of dollars).

#### **Details**

The data is taken from the National Bureau of Economic Research R\&D Masterfile.

## **Source**

P. Wang, I.M. Cockburn and M.L. Puterman. Analysis of Patent Data – A Mixed-Poisson-Regression-Model Approach. *Journal of Business & Economic Statistics*, **16**(1), 27–41, 1998.

## References

B.H. Hall, C. Cummins, E. Laderman and J. Mundy. The R&D Master File Documentation. Technical Working Paper 72, National Bureau of Economic Research, 1988. Cambridge, MA.

# Examples

plot-methods

Rootogram of Posterior Probabilities

## **Description**

The plot method for flexmix-class objects gives a rootogram or histogram of the posterior probabilities.

# Usage

```
## S4 method for signature 'flexmix,missing'
plot(x, y, mark = NULL, markcol = NULL,
  col = NULL, eps = 1e-4, root = TRUE, ylim = TRUE, main = NULL, xlab = "",
  ylab = "", as.table = TRUE, endpoints = c(-0.04, 1.04), ...)
```

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#### **Arguments**

x An object of class "flexmix".

y Not used.

mark Integer: mark posteriors of this component.

markcol Color used for marking components.

col Color used for the bars.

eps Posteriors smaller than eps are ignored.

root If TRUE, a rootogram of the posterior probabilities is drawn, otherwise a standard

histogram.

ylim A logical value or a numeric vector of length 2. If TRUE, the y axes of all

rootograms are aligned to have the same limits, if FALSE each y axis is scaled

separately. If a numeric vector is specified it is used as usual.

main Main title of the plot.

xlab Label of x-axis. ylab Label of y-axis.

as.table Logical that controls the order in which panels should be plotted: if FALSE (the

default), panels are drawn left to right, bottom to top (as in a graph); if TRUE, left

to right, top to bottom.

endpoints Vector of length 2 indicating the range of x-values that is to be covered by the

histogram. This applies only when breaks is unspecified. In do.breaks, this

specifies the interval that is to be divided up.

... Further graphical parameters for the lattice function histogram.

## **Details**

For each mixture component a rootogram or histogram of the posterior probabilities of all observations is drawn. Rootograms are very similar to histograms, the only difference is that the height of the bars correspond to square roots of counts rather than the counts themselves, hence low counts are more visible and peaks less emphasized. Please note that the y-axis denotes the number of observations in each bar in any case.

Usually in each component a lot of observations have posteriors close to zero, resulting in a high count for the corresponding bin in the rootogram which obscures the information in the other bins. To avoid this problem, all probabilities with a posterior below eps are ignored.

A peak at probability one indicates that a mixture component is well seperated from the other components, while no peak at one and/or significant mass in the middle of the unit interval indicates overlap with other components.

#### Author(s)

Friedrich Leisch and Bettina Gruen

plotEll 53

## References

Friedrich Leisch. FlexMix: A general framework for finite mixture models and latent class regression in R. *Journal of Statistical Software*, **11**(8), 2004. http://www.jstatsoft.org/v11/i08/

Jeremy Tantrum, Alejandro Murua and Werner Stuetzle. Assessment and pruning of hierarchical model based clustering. Proceedings of the 9th ACM SIGKDD international conference on Knowledge Discovery and Data Mining, 197–205. ACM Press, New York, NY, USA, 2003.

Friedrich Leisch. Exploring the structure of mixture model components. In Jaromir Antoch, editor, Compstat 2004–Proceedings in Computational Statistics, 1405–1412. Physika Verlag, Heidelberg, Germany, 2004. ISBN 3-7908-1554-3.

plotEll

Plot Confidence Ellipses for FLXMCmvnorm Results

## Description

Plot 50% and 95% confidence ellipses for mixtures of Gaussians fitted using FLXMCmvnorm.

## Usage

## **Arguments**

object	An object of class flexmix with a fitted FLXMCmvnorm model.
data	The response variable in a data frame or as a matrix.
which	Index numbers of dimensions of (projected) input space to plot.
model	The model (for a multivariate response) that shall be plotted.
project	Projection object, currently only the result of prcomp is supported.
points	Logical, shall data points be plotted?
eqscale	Logical, plot using eqscplot?
number	Logical, plot number labels at cluster centers?
cex, numcol	Size and color of number labels.
pch, col,	Graphical parameters.

## Author(s)

Friedrich Leisch and Bettina Gruen

## See Also

FLXMCmvnorm

54 refit-methods

posterior

Determine Cluster Membership and Posterior Probabilities

## **Description**

Determine posterior probabilities or cluster memberships for a fitted flexmix or unfitted FLXdist model.

## Usage

```
## S4 method for signature 'flexmix,missing'
posterior(object, newdata, unscaled = FALSE, ...)
## S4 method for signature 'FLXdist,listOrdata.frame'
posterior(object, newdata, unscaled = FALSE, ...)
## S4 method for signature 'flexmix,missing'
clusters(object, newdata, ...)
## S4 method for signature 'FLXdist,ANY'
clusters(object, newdata, ...)
```

# **Arguments**

object An object of class "flexmix" or "FLXdist".

Data frame or list containing new data. If missing the posteriors of the original observations are returned.

Logical, if TRUE the component-specific likelihoods are returned.

... Currently not used.

## Author(s)

Friedrich Leisch and Bettina Gruen

refit-methods

Refit a Fitted Model

# Description

Refits an estimated flexmix model to obtain additional information like coefficient significance p-values for GLM regression.

refit-methods 55

## **Usage**

## **Arguments**

object An object of class "flexmix"

newdata Optional new data.

method Specifies if the variance covariance matrix is determined using optim or if the

posteriors are assumed as given and an M-step is performed.

model The model (for a multivariate response) that shall be used.

which Specifies if a component specific model or the concomitant variable model is

used.

x An object of class "FLXRoptim"

y Missing object.

bycluster A logical if the parameters should be group by cluster or by variable.

alpha Numeric indicating the significance level.

components Numeric vector specifying which components are plotted. The default is to plot

all components.

labels Character vector specifying the variable names used.

significance A logical indicating if non-significant coefficients are shaded in a lighter grey.

xlab String for the x-axis label. ylab String for the y-axis label.

ci A logical indicating if significant and insignificant parameter estimates are shaded

differently.

scales See argument of the same name for function xyplot.

as.table See arguments of the same name for function xyplot.

horizontal See arguments of the same name for function xyplot.

... Currently not used

56 refit-methods

#### **Details**

The refit method for FLXMRglm models in combination with the summary method can be used to obtain the usual tests for significance of coefficients. Note that the tests are valid only if flexmix returned the maximum likelihood estimator of the parameters. If refit is used with method = "mstep" for these component specific models the returned object contains a glm object for each component where the elements model which is the model frame and data which contains the original dataset are missing.

#### Value

An object inheriting form class FLXR is returned. For the method using optim the object has class FLXRoptim and for the M-step method it has class FLXRmstep. Both classes give similar results for their summary methods. Objects of class FLXRoptim have their own plot method. Lapply can be used to further analyse the refitted component specific models of objects of class FLXRmstep.

#### Warning

For method = "mstep" the standard deviations are determined separately for each of the components using the a-posteriori probabilities as weights without accounting for the fact that the components have been simultaneously estimated. The derived standard deviations are hence approximative and should only be used in an exploratory way, as they are underestimating the uncertainty given that the missing information of the component memberships are replaced by the expected values.

The newdata argument can only be specified when using method = "mstep" for refitting FLXMRglm components. A variant of glm for weighted ML estimation is used for fitting the components and full glm objects are returned. Please note that in this case the data and the model frame are stored for each component which can significantly increase the object size.

#### Author(s)

Friedrich Leisch and Bettina Gruen

#### References

Friedrich Leisch. FlexMix: A general framework for finite mixture models and latent class regression in R. *Journal of Statistical Software*, **11**(8), 2004. http://www.jstatsoft.org/v11/i08/

```
data("NPreg", package = "flexmix")
ex1 <- flexmix(yn ~ x + I(x^2), data = NPreg, k = 2)
ex1r <- refit(ex1)

## in one component all coefficients should be highly significant,
## in the other component only the linear term
summary(ex1r)</pre>
```

relabel 57

relabel

Relabel the Components

## **Description**

The components are sorted by the value of one of the parameters or according to an integer vector containing the permutation of the numbers from 1 to the number of components.

## Usage

```
relabel(object, by, ...)
## S4 method for signature 'FLXdist,character'
relabel(object, by, which = NULL, ...)
```

# Arguments

object	An object of class "flexmix".
by	If a character vector, it needs to be one of "prior", "model", "concomitant" indicating if the parameter should be from the component-specific or the concomitant variable model. If an integer vector it indicates how the components should be sorted. If missing, the components are sorted by component size.
which	Name (or unique substring) of a parameter if by is equal to "model" or "concomitant".
	Currently not used.

## Author(s)

Friedrich Leisch and Bettina Gruen

```
set.seed(123)
beta <- matrix(1:16, ncol = 4)
beta
df1 <- ExLinear(beta, n = 100, sd = .5)
f1 <- flexmix(y~., data = df1, k = 4)

## There was label switching, parameters are not in the same order
## as in beta:
round(parameters(f1))

betas <- rbind(beta, .5)
betas

## This makes no sense:
summary(abs(as.vector(betas-parameters(f1))))

## We relabel the components by sorting the coefficients of x1:</pre>
```

58 rflexmix

```
r1 <- relabel(f1, by = "model", which = "x1")
round(parameters(r1))
## Now we can easily compare the fit with the true parameters:
summary(abs(as.vector(betas-parameters(r1))))</pre>
```

rflexmix

Random Number Generator for Finite Mixtures

# Description

Given a finite mixture model generate random numbers from it.

# Usage

```
rflexmix(object, newdata, ...)
```

## **Arguments**

object A fitted finite mixture model of class flexmix or an unfitted of class FLXdist.

newdata Optionally, a data frame in which to look for variables with which to predict or

an integer specifying the number of random draws for model-based clustering.

If omitted, the data to which the model was fitted is used.

... Further arguments to be passed to or from methods.

## **Details**

rflexmix provides the creation of the model matrix for new data and the sampling of the cluster memberships. The sampling of the component distributions given the classification is done by calling rFLXM. This step has to be provided for the different model classes.

## Value

A list with components

y Random sample group Grouping factor class Class membership

## Author(s)

Bettina Gruen

```
example(flexmix)
sample <- rflexmix(ex1)</pre>
```

salmonellaTA98 59

salmonellaTA98

Salmonella Reverse Mutagenicity Assay

## **Description**

Data on Ames Salmonella reverse mutagenicity assay.

## Usage

```
data("salmonellaTA98")
```

#### **Format**

This data frame contains the following columns:

- x Dose levels of quinoline.
- y Numbers of revertant colonies of TA98 Salmonella observed on each of three replicate plates tested at each of six dose levels of quinoline diameter.

#### **Details**

This data set is taken from package **dispmod** provided by Luca Scrucca.

#### **Source**

Margolin, B.J., Kaplan, N. and Zeiger, E. Statistical analysis of the Ames Salmonella/microsome test, *Proc. Natl. Acad. Sci. USA*, **76**, 3779–3783, 1981.

## References

Breslow, N.E. Extra-Poisson variation in log-linear models, Applied Statistics, 33, 38-44, 1984.

Wang, P., Puterman, M.L., Cockburn, I.M., and Le, N.D. Mixed Poisson regression models with covariate dependent rates, *Biometrics*, **52**, 381–400, 1996.

60 seizure

seizure

Epileptic Seizure Data

## **Description**

Data from a clinical trial where the effect of intravenous gamma-globulin on suppression of epileptic seizures is studied. Daily observations for a period of 140 days on one patient are given, where the first 27 days are a baseline period without treatment, the remaining 113 days are the treatment period.

## Usage

```
data("seizure")
```

#### **Format**

A data frame with 140 observations on the following 4 variables.

**Seizures** A numeric vector, daily counts of epileptic seizures.

**Hours** A numeric vector, hours of daily parental observation.

**Treatment** A factor with levels No and Yes.

Day A numeric vector.

#### Source

P. Wang, M. Puterman, I. Cockburn, and N. Le. Mixed poisson regression models with covariate dependent rates. *Biometrics*, **52**, 381–400, 1996.

## References

B. Gruen and F. Leisch. Bootstrapping finite mixture models. In J. Antoch, editor, Compstat 2004–Proceedings in Computational Statistics, 1115–1122. Physika Verlag, Heidelberg, Germany, 2004. ISBN 3-7908-1554-3.

stepFlexmix 61

stepFlexmix

Run FlexMix Repeatedly

## **Description**

Runs flexmix repeatedly for different numbers of components and returns the maximum likelihood solution for each.

## Usage

## Arguments

... Passed to flexmix (or matplot in the plot method).

k A vector of integers passed in turn to the k argument of flexmix.

init An object of class "initMethod" or a named list where initMethod is called

with it as arguments in addition to the control argument.

62 stepFlexmix

name	A character string indication which initialization strategy should be employed: short runs of EM followed by a long ("tol.em"), short runs of CEM followed by a long EM run ("cem.em"), short runs of SEM followed by a long EM run ("sem.em").
step1	A named list which combined with the control argument is coercable to a "FLXcontrol" object. This control setting is used for the short runs.
step2	A named list which combined with the control argument is coercable to a "FLXcontrol" object. This control setting is used for the long run.
control	A named list which combined with the step1 or the step2 argument is coercable to a "FLXcontrol" object.
nrep	For each value of k run flexmix nrep times and keep only the solution with maximum likelihood. If nrep is set for the long run, it is ignored, because the EM algorithm is deterministic using the best solution discovered in the short runs for initialization.
verbose	If TRUE, show progress information during computations.
drop	If TRUE and k is of length 1, then a single flexmix object is returned instead of a "stepFlexmix" object.
unique	If TRUE, then unique() is called on the result, see below.
x, object	An object of class "stepFlexmix".
У	Not used.
what	Character vector naming information criteria to plot. Functions of the same name must exist, which take a stepFlexmix object as input and return a numeric vector like AIC, stepFlexmix-method (see examples below).
xlab,ylab	Graphical parameters.
legend	If not FALSE and what contains more than 1 element, a legend is placed at the specified location, see legend for details.
which	Number of model to get. If character, interpreted as number of components or name of an information criterion.
incomparables	A vector of values that cannot be compared. Currently, FALSE is the only possible value, meaning that all values can be compared.

## Value

An object of class "stepFlexmix" containing the best models with respect to the log likelihood for the different number of components in a slot if length(k)>1, else directly an object of class "flexmix".

If unique = FALSE, then the resulting object contains one model per element of k (which is the number of clusters the EM algorithm started with). If unique = TRUE, then the result is resorted according to the number of clusters contained in the fitted models (which may be less than the number with which the EM algorithm started), and only the maximum likelihood solution for each number of fitted clusters is kept. This operation can also be done manually by calling unique() on objects of class "stepFlexmix".

stepFlexmix 63

## Author(s)

Friedrich Leisch and Bettina Gruen

#### References

Friedrich Leisch. FlexMix: A general framework for finite mixture models and latent class regression in R. *Journal of Statistical Software*, **11**(8), 2004. http://www.jstatsoft.org/v11/i08/

Christophe Biernacki, Gilles Celeux and Gerard Govaert. Choosing starting values for the EM algorithm for getting the highest likelihood in multivariate Gaussian mixture models. *Computational Statistics & Data Analysis*, **41**(3–4), 561–575, 2003.

Theresa Scharl, Bettina Gruen and Friedrich Leisch. Mixtures of regression models for time-course gene expression data: Evaluation of initialization and random effects. *Bioinformatics*, **26**(3), 370–377, 2010.

```
data("Nclus", package = "flexmix")
## try 2 times for k = 4
set.seed(511)
ex1 <- initFlexmix(Nclus~1, k = 4, model = FLXMCmvnorm(diagonal = FALSE),
                   nrep = 2)
ex1
## now 2 times each for k = 2:5, specify control parameter
ex2 <- initFlexmix(Nclus~1, k = 2:5, model = FLXMCmvnorm(diagonal = FALSE),
                   control = list(minprior = 0), nrep = 2)
ex2
plot(ex2)
## get BIC values
BIC(ex2)
## get smallest model
getModel(ex2, which = 1)
## get model with 3 components
getModel(ex2, which = "3")
## get model with smallest ICL (here same as for AIC and BIC: true k = 4)
getModel(ex2, which = "ICL")
## now 1 time each for k = 2:5, with larger minimum prior
ex3 <- initFlexmix(Nclus~1, k = 2:5,
                   model = FLXMCmvnorm(diagonal = FALSE),
                   control = list(minprior = 0.1), nrep = 1)
ex3
## keep only maximum likelihood solution for each unique number of
## fitted clusters:
unique(ex3)
```

64 tribolium

tribolium

Tribolium Beetles

# Description

The data investigates whether the adult Tribolium species Castaneum has developed an evolutionary advantage to recognize and avoid eggs of their own species while foraging.

## Usage

```
data("tribolium")
```

#### **Format**

A data frame with 27 observations on the following 4 variables.

Remaining A numeric vector.

Total A numeric vector.

Replicate A factor with levels 1, 2, 3.

Species A factor with levels Castaneum Confusum Madens.

#### **Details**

Beetles of the genus Tribolium are cannibalistic in the sense that adults eat the eggs of their own species as well as those of closely related species. The experiment isolated a number of adult beetles of the same species and presented them with a vial of 150 eggs (50 of each type), the eggs being thoroughly mixed to ensure uniformity throughout the vial.

The data gives the consumption data for adult Castaneum species. It reports the number of Castaneum, Confusum and Madens eggs, respectively, that remain uneaten after two day exposure to the adult beetles. Replicates 1, 2, and 3 correspond to different occasions on which the experiment was conducted.

#### Source

P. Wang and M.L. Puterman. Mixed Logistic Regression Models. *Journal of Agricultural, Biological, and Environmental Statistics*, **3** (2), 175–200, 1998.

trypanosome 65

trypanosome

Trypanosome

## Description

Trypanosome data from a dosage-response analysis to assess the proportion of organisms belonging to different populations. It is assumed that organisms belonging to different populations are indistinguishable other than in terms of their reaction to the stimulus.

# Usage

```
data("trypanosome")
```

#### **Format**

A data frame with 426 observations on the following 2 variables.

Dead A logical vector.

Dose A numeric vector.

## **Details**

The experimental technique involved inspection under the microscope of a representative aliquot of a suspension, all organisms appearing within two fields of view being classified either alive or dead. Hence the total numbers of organisms present at each dose and the number showing the quantal response were both random variables.

#### Source

R. Ashford and P.J. Walker. Quantal Response Analysis for a Mixture of Populations. *Biometrics*, **28**, 981–988, 1972.

## References

D.A. Follmann and D. Lambert. Generalizing Logistic Regression by Nonparametric Mixing. *Journal of the American Statistical Association*, **84**(405), 195–300, 1989.

66 whiskey

whiskey

Survey Data on Brands of Scotch whiskey Consumed

## **Description**

The data set is from Simmons Study of Media and Markets and contains the incidence matrix for scotch brands used in last year for those households who report consuming scotch.

#### **Usage**

```
data("whiskey")
```

## **Format**

A data frame whiskey with 484 observations on the following 2 variables.

Freq a numeric vector

Incidence a matrix with 21 columns

Additional information on the brands is contained in the data frame whiskey\_brands which is simultaneously loaded. This data frame contains 21 observations on the following 3 variables.

Brand a character vector

Type a factor with levels Blend Single Malt

Bottled a factor with levels Domestic Foreign

## **Details**

The dataset is taken from the **bayesm** package.

## Source

Peter Rossi and Rob McCulloch. bayesm: Bayesian Inference for Marketing/Micro-econometrics. R package version 2.0-8, 2006. http://gsbwww.uchicago.edu/fac/peter.rossi/research/bsm.html

#### References

Edwards, Y. and G. Allenby. Multivariate Analysis of Multiple Response Data, *Journal of Marketing Research*, **40**, 321–334, 2003.

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