Package 'mclust'

March 31, 2016

version 5.2
Date 2016-03-22
Title Gaussian Mixture Modelling for Model-Based Clustering, Classification, and Density Estimation
Description Gaussian finite mixture models fitted via EM algorithm for model-based clustering, class sification, and density estimation, including Bayesian regularization, dimension reduction for visualisation, and resampling-based inference.
Depends R (>= 3.0)
Imports stats, utils, graphics, grDevices
Suggests knitr (>= 1.12), rmarkdown (>= 0.9), mix (>= 1.0)
License GPL (>= 2)
<pre>URL http://www.stat.washington.edu/mclust/</pre>
VignetteBuilder knitr
Repository CRAN
ByteCompile true
LazyLoad yes
NeedsCompilation yes
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Date/Publication 2016-03-31 17:39:13
R topics documented:
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mclust-package	Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation
	and 2 charly Estimation

Description

Finite Gaussian mixture modeling fitted via EM algorithm for model-based clustering, classification, and density estimation, including Bayesian regularization and dimension reduction.

Details

For a quick introduction to **mclust** see the vignette A quick tour of mclust.

References

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611:631*.

Author(s)

Chris Fraley, Adrian Raftery and Luca Scrucca.

Maintainer: Luca Scrucca < luca@stat.unipg.it>

```
# Clustering
mod1 = Mclust(iris[,1:4])
summary(mod1)
plot(mod1, what = c("BIC", "classification"))
# Classification
data(banknote)
mod2 = MclustDA(banknote[,2:7], banknote$Status)
summary(mod2)
plot(mod2)
# Density estimation
mod3 = densityMclust(faithful$waiting)
summary(mod3)
plot(mod3, faithful$waiting)
```

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acidity Acidity data

Description

Acidity index measured in a sample of 155 lakes in the Northeastern United States. The data are on the log scale, as analysed by Crawford et al. (1992, 1994). The data were also used to fit mixture of gaussian distributions by Richardson and Green (1997), and by McLachlan and Peel (2000, Sec. 6.6.2).

Usage

data(acidity)

Source

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

References

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

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

McLachlan, G. and Peel, D. (2000) Finite Mixture Models. Wiley, New York.

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

Description

Computes the adjusted Rand index comparing two classifications.

Usage

```
adjustedRandIndex(x, y)
```

Arguments

x A numeric or character vector of class labels.

y A numeric or character vector of class labels. The length of y should be the same as that of x.

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Value

The adjusted Rand index comparing the two partitions (a scalar). This index has zero expected value in the case of random partition, and it is bounded above by 1 in the case of perfect agreement between two partitions.

References

L. Hubert and P. Arabie (1985) Comparing Partitions, Journal of the Classification 2:193-218.

See Also

```
classError, mapClass, table
```

Examples

```
a <- rep(1:3, 3)
a
b <- rep(c("A", "B", "C"), 3)
b
adjustedRandIndex(a, b)

a <- sample(1:3, 9, replace = TRUE)
a
b <- sample(c("A", "B", "C"), 9, replace = TRUE)
b
adjustedRandIndex(a, b)

a <- rep(1:3, 4)
a
b <- rep(c("A", "B", "C", "D"), 3)
b
adjustedRandIndex(a, b)

irisHCvvv <- hc(modelName = "VVV", data = iris[,-5])
cl3 <- hclass(irisHCvvv, 3)
adjustedRandIndex(cl3,iris[,5])

irisBIC <- mclustBIC(iris[,-5])
adjustedRandIndex(summary(irisBIC,iris[,-5],$classification,iris[,5])
adjustedRandIndex(summary(irisBIC,iris[,-5],G=3)$classification,iris[,5])
adjustedRandIndex(summary(irisBIC,iris[,-5],G=3)$classification,iris[,5])</pre>
```

banknote

Swiss banknotes data

Description

The data set contains six measurements made on 100 genuine and 100 counterfeit old-Swiss 1000-franc bank notes.

Usage

data(banknote)

Format

A data frame with the following variables:

Status the status of the banknote: genuine or counterfeit

Length Length of bill (mm)

Left Width of left edge (mm)

Right Width of right edge (mm)

Bottom Bottom margin width (mm)

Top Top margin width (mm)

Diagonal Length of diagonal (mm)

Source

Flury, B. and Riedwyl, H. (1988). *Multivariate Statistics: A practical approach*. London: Chapman & Hall, Tables 1.1 and 1.2, pp. 5-8.

Baudry_etal_2010_JCGS_examples

Simulated Example Datasets From Baudry et al. (2010)

Description

Simulated datasets used in Baudry et al. (2010) to illustrate the proposed mixture components combining method for clustering.

Please see the cited article for a detailed presentation of these datasets. The data frame with name exN.M is presented in Section N.M in the paper.

Test1D (not in the article) has been simulated from a Gaussian mixture distribution in R.

ex4.1 and ex4.2 have been simulated from a Gaussian mixture distribution in R^2.

ex4.3 has been simulated from a mixture of a uniform distribution on a square and a spherical Gaussian distribution in R^2.

ex4.4.1 has been simulated from a Gaussian mixture model in R^2

ex4.4.2 has been simulated from a mixture of two uniform distributions in R³.

Usage

```
data(Baudry_etal_2010_JCGS_examples)
```

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Format

```
ex4.1 is a data frame with 600 observations on 2 real variables.
ex4.2 is a data frame with 600 observations on 2 real variables.
ex4.3 is a data frame with 200 observations on 2 real variables.
ex4.4.1 is a data frame with 800 observations on 2 real variables.
ex4.4.2 is a data frame with 300 observations on 3 real variables.
Test1D is a data frame with 200 observations on 1 real variable.
```

References

J.-P. Baudry, A. E. Raftery, G. Celeux, K. Lo and R. Gottardo (2010). Combining mixture components for clustering. *Journal of Computational and Graphical Statistics*, 19(2):332-353.

Examples

```
## Not run:
data(Baudry_etal_2010_JCGS_examples)

output <- clustCombi(ex4.4.1)

output # is of class clustCombi

# plots the hierarchy of combined solutions, then some "entropy plots" which # may help one to select the number of classes plot(output, ex4.4.1)

## End(Not run)</pre>
```

bic

BIC for Parameterized Gaussian Mixture Models

Description

Computes the BIC (Bayesian Information Criterion) for parameterized mixture models given the loglikelihood, the dimension of the data, and number of mixture components in the model.

Usage

```
bic(modelName, loglik, n, d, G, noise=FALSE, equalPro=FALSE, ...)
```

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Arguments

modelName	A character string indicating the model. The help file for mclustModelNames describes the available models.
loglik	The log-likelihood for a data set with respect to the Gaussian mixture model specified in the modelName argument.
n	The number of observations in the data used to compute loglik.
d	The dimension of the data used to compute loglik.
G	The number of components in the Gaussian mixture model used to compute loglik.
noise	A logical variable indicating whether or not the model includes an optional Poisson noise component. The default is to assume no noise component.
equalPro	A logical variable indicating whether or not the components in the model are assumed to be present in equal proportion. The default is to assume unequal mixing proportions.
	Catches unused arguments in an indirect or list call via do.call.

Value

The BIC or Bayesian Information Criterion for the given input arguments.

References

C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611:631*.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

mclustBIC, nVarParams, mclustModelNames.

```
n <- nrow(iris)
d <- ncol(iris)-1
G <- 3

emEst <- me(modelName="VVI", data=iris[,-5], unmap(iris[,5]))
names(emEst)

args(bic)
bic(modelName="VVI", loglik=emEst$loglik, n=n, d=d, G=G)
## Not run: do.call("bic", emEst) ## alternative call</pre>
```

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cdens

Component Density for Parameterized MVN Mixture Models

Description

Computes component densities for observations in MVN mixture models parameterized by eigenvalue decomposition.

Usage

```
cdens(modelName, data, logarithm = FALSE, parameters, warn = NULL, ...)
```

Arguments

6	
modelName	A character string indicating the model. The help file for ${\tt mclustModelNames}$ describes the available models.
data	A numeric vector, matrix, or data frame of observations. Categorical variables are not allowed. If a matrix or data frame, rows correspond to observations and columns correspond to variables.
logarithm	A logical value indicating whether or not the logarithm of the component densities should be returned. The default is to return the component densities, obtained from the log component densities by exponentiation.
parameters	The parameters of the model:
	mean The mean for each component. If there is more than one component, this is a matrix whose kth column is the mean of the k th component of the mixture model.
	variance A list of variance parameters for the model. The components of this list depend on the model specification. See the help file for mclustVariance for details.
warn	A logical value indicating whether or not a warning should be issued when computations fail. The default is warn=FALSE.
	Catches unused arguments in indirect or list calls via do.call.

Value

A numeric matrix whose [i,k]th entry is the density or log density of observation i in component k. The densities are not scaled by mixing proportions.

References

- C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611-631*.
- C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

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Note

When one or more component densities are very large in magnitude, it may be possible to compute the logarithm of the component densities but not the component densities themselves due to overflow.

See Also

```
\verb|cdensE|, \dots, \verb|cdensVVV|, \verb|dens|, \verb|estep|, \verb|mclustModelNames|, \verb|mclustVariance|, \verb|mclust.options|, \verb|do.call|| \\
```

Examples

cdensE

Component Density for a Parameterized MVN Mixture Model

Description

Computes component densities for points in a parameterized MVN mixture model.

Usage

```
cdensE(data, logarithm = FALSE, parameters, warn = NULL, ...)
cdensV(data, logarithm = FALSE, parameters, warn = NULL, ...)
cdensX(data, logarithm = FALSE, parameters, warn = NULL, ...)
cdensEII(data, logarithm = FALSE, parameters, warn = NULL, ...)
cdensVII(data, logarithm = FALSE, parameters, warn = NULL, ...)
cdensEEI(data, logarithm = FALSE, parameters, warn = NULL, ...)
cdensVEI(data, logarithm = FALSE, parameters, warn = NULL, ...)
cdensEVI(data, logarithm = FALSE, parameters, warn = NULL, ...)
cdensVVI(data, logarithm = FALSE, parameters, warn = NULL, ...)
cdensEEE(data, logarithm = FALSE, parameters, warn = NULL, ...)
```

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```
cdensEEV(data, logarithm = FALSE, parameters, warn = NULL, ...)
cdensVEV(data, logarithm = FALSE, parameters, warn = NULL, ...)
cdensVVV(data, logarithm = FALSE, parameters, warn = NULL, ...)
cdensEVE(data, logarithm = FALSE, parameters, warn = NULL, ...)
cdensEVV(data, logarithm = FALSE, parameters, warn = NULL, ...)
cdensVEE(data, logarithm = FALSE, parameters, warn = NULL, ...)
cdensVVE(data, logarithm = FALSE, parameters, warn = NULL, ...)
cdensXII(data, logarithm = FALSE, parameters, warn = NULL, ...)
cdensXXX(data, logarithm = FALSE, parameters, warn = NULL, ...)
```

Arguments

A numeric vector, matrix, or data frame of observations. Categorical variables are not allowed. If a matrix or data frame, rows correspond to observations and

columns correspond to variables.

logarithm A logical value indicating whether or not the logarithm of the component den-

sities should be returned. The default is to return the component densities, ob-

tained from the log component densities by exponentiation.

parameters The parameters of the model:

mean The mean for each component. If there is more than one component, this is a matrix whose kth column is the mean of the *k*th component of the mixture model.

variance A list of variance parameters for the model. The components of this list depend on the model specification. See the help file for mclustVariance for details.

pro Mixing proportions for the components of the mixture. If the model includes a Poisson term for noise, there should be one more mixing proportion than the number of Gaussian components.

warn A logical value indicating whether or not a warning should be issued when com-

putations fail. The default is warn=FALSE.

. . . Catches unused arguments in indirect or list calls via do.call.

Value

A numeric matrix whose [i,j]th entry is the density of observation i in component j. The densities are not scaled by mixing proportions.

References

C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611-631*.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

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Note

When one or more component densities are very large in magnitude, then it may be possible to compute the logarithm of the component densities but not the component densities themselves due to overflow.

See Also

```
cdens, dens, mclustVariance, mstep, mclust.options, do.call.
```

Examples

```
z2 <- unmap(hclass(hcVVV(faithful),2)) # initial value for 2 class case
model <- meVVV(data=faithful, z=z2)
cdensVVV(data=faithful, logarithm = TRUE, parameters = model$parameters)
data(cross)
z2 <- unmap(cross[,1])
model <- meEEV(data = cross[,-1], z = z2)
EEVdensities <- cdensEEV( data = cross[,-1], parameters = model$parameters)
cbind(cross[,-1],map(EEVdensities))</pre>
```

cdfMclust

Cumulative Distribution and Quantiles for a univariate Gaussian mixture distribution

Description

Compute the cumulative density function (cdf) or quantiles from an estimated one-dimensional Gaussian mixture fitted using densityMclust.

Usage

```
cdfMclust(object, data, ngrid = 100, ...)
quantileMclust(object, p, ...)
```

Arguments

object	a densityMclust model object.
data	a numeric vector of evaluation points.
ngrid	the number of points in a regular grid to be used as evaluation points if no data are provided.
p	a numeric vector of probabilities.
	further arguments passed to or from other methods.

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Details

The cdf is evaluated at points given by the optional argument data. If not provided, a regular grid of length ngrid for the evaluation points is used.

The quantiles are computed using interpolating splines on an adaptive finer grid.

Value

cdfMclust returns a list of x and y values providing, respectively, the evaluation points and the estimated cdf.

quantileMclust returns a vector of quantiles.

References

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

Author(s)

Luca Scrucca

See Also

```
densityMclust, plot.densityMclust.
```

```
x \leftarrow c(rnorm(100), rnorm(100, 3, 2))
dens <- densityMclust(x)</pre>
summary(dens, parameters = TRUE)
cdf <- cdfMclust(dens)</pre>
str(cdf)
q \leftarrow quantileMclust(dens, p = c(0.01, 0.1, 0.5, 0.9, 0.99))
cbind(quantile = q, cdf = cdfMclust(dens, q)$y)
plot(cdf, type = "1", xlab = "x", ylab = "CDF")
points(q, cdfMclust(dens, q)$y, pch = 20, col = "red3")
par(mfrow = c(2,2))
dens.waiting <- densityMclust(faithful$waiting)</pre>
plot(dens.waiting)
plot(cdfMclust(dens.waiting), type = "l",
     xlab = dens.waiting$varname, ylab = "CDF")
dens.eruptions <- densityMclust(faithful$eruptions)</pre>
plot(dens.eruptions)
plot(cdfMclust(dens.eruptions), type = "1",
     xlab = dens.eruptions$varname, ylab = "CDF")
par(mfrow = c(1,1))
```

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chevron

Simulated minefield data

Description

A set of simulated bivariate minefield data (1104 observations).

Usage

data(chevron)

References

- A. Dasgupta and A. E. Raftery (1998). Detecting features in spatial point processes with clutter via model-based clustering. *Journal of the American Statistical Association 93:294-302*.
- C. Fraley and A.E. Raftery (1998). Computer Journal 41:578-588.
- G. J. McLachlan and D. Peel (2000). Finite Mixture Models, Wiley, pages 110-112.

classError

Classification error

Description

Error for a given classification relative to a known truth. Location of errors in a given classification relative to a known truth.

Usage

```
classError(classification, truth)
```

Arguments

classification A numeric or character vector of class labels.

truth A numeric or character vector of class labels. Must have the same length as

classification.

Details

If more than one mapping between classification and truth corresponds to the minimum number of classification errors, only one possible set of misclassified observations is returned.

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Value

A list with the following two components:

misclassified The indexes of the misclassified data points in a minimum error mapping between the given classification and the given truth.

errorRate The errorRate corresponding to a minimum error mapping mapping between the given classification and the given truth.

References

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

```
mapClass, table
```

Examples

```
a <- rep(1:3, 3)
a
b <- rep(c("A", "B", "C"), 3)
b
classError(a, b)

a <- sample(1:3, 9, replace = TRUE)
a
b <- sample(c("A", "B", "C"), 9, replace = TRUE)
b
classError(a, b)</pre>
```

clPairs

Pairwise Scatter Plots showing Classification

Description

Creates a scatter plot for each pair of variables in given data. Observations in different classes are represented by different colors and symbols.

Usage

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Arguments

data	A numeric vector, matrix, or data frame of observations. Categorical variables are not allowed. If a matrix or data frame, rows correspond to observations and columns correspond to variables.
classification	A numeric or character vector representing a classification of observations (rows) of data.
symbols	Either an integer or character vector assigning a plotting symbol to each unique class in classification. Elements in symbols correspond to classes in order of appearance in the sequence of observations (the order used by the function unique). The default is given by mclust.options("classPlotSymbols").
colors	Either an integer or character vector assigning a color to each unique class in classification. Elements in colors correspond to classes in order of appearance in the sequence of observations (the order used by the function unique). The default is given by mclust.options("classPlotColors").
labels	A vector of character strings for labeling the variables. The default is to use the column dimension names of data.
CEX	An argument specifying the size of the plotting symbols. The default value is 1.
gap	An argument specifying the distance between subplots (see pairs).
х,у	The x and y co-ordinates with respect to a graphic device having plotting region coordinates $par("usr" = c(0,1,0,1))$.
class	The class labels.
col, pch	The colors and plotting symbols appearing in the legend.
	For a clPairs call may be additional arguments to be passed to pairs. For a clPairsLegend call may be additional arguments to be passed to legend.

Value

The function clPairs invisibly returns a list with the following components:

class A character vector of class labels.

col A vector of colors used for each class.

pch A vector of plotting symbols used for each class.

Details

The function clPairs draws scatter plots on the current graphics device for each combination of variables in data. Observations of different classifications are labeled with different symbols.

The function clPairsLegend can be used to add a legend. See examples below.

References

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

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See Also

```
pairs, coordProj, mclust.options
```

Examples

clustCombi

Combining Gaussian Mixture Components for Clustering

Description

Provides a hierarchy of combined clusterings from the EM/BIC Gaussian mixture solution to one class, following the methodology proposed in the article cited in the references.

Usage

```
clustCombi(data, MclustOutput = NULL, ...)
```

Arguments

data

A numeric vector, matrix, or data frame of observations. Categorical variables are not allowed. If a matrix or data frame, rows correspond to observations and columns correspond to variables.

MclustOutput

A list giving the optimal (according to BIC) parameters, conditional probabilities z, and log-likelihood, together with the associated classification and its uncertainty, as returned by Mclust. Please see Mclust documentation for the details of the components. Default value is NULL, in which case Mclust is called to get this output.

. . .

Optional arguments to be passed to called functions. Notably, any option (such as the numbers of components for which the BIC is computed; the models to be fitted by EM; initialization parameters for the EM algorithm...) to be passed to Mclust in case MclustOutput is NULL. Please see the Mclust documentation for more details.

Details

Mclust provides a Gaussian mixture fitted to the data by maximum likelihood through the EM algorithm, for the model and number of components selected according to BIC. The corresponding components are hierarchically combined according to an entropy criterion, following the methodology described in the article cited in the references section. The solutions with numbers of classes between the one selected by BIC and one are returned as a clustCombi class object.

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Value

A list of class clustCombi giving the hierarchy of combined solutions from the number of components selected by BIC to one. The details of the output components are as follows:

classification A list of the data classifications obtained for each combined solution of the hi-

erarchy through a MAP assignment

combiM A list of matrices. combiM[[K]] is the matrix used to combine the components

of the (K+1)-classes solution to get the K-classes solution. Please see the exam-

ples.

combiz A list of matrices. combiz[[K]] is a matrix whose [i,k]th entry is the probability

that observation i in the data belongs to the kth class according to the K-classes

combined solution.

MclustOutput A list of class Mclust. Output of a call to the Mclust function (as provided by the

user or the result of a call to the Mclust function) used to initiate the combined solutions hierarchy: please see the Mclust function documentation for details.

Author(s)

J.-P. Baudry, A. E. Raftery, L. Scrucca

References

J.-P. Baudry, A. E. Raftery, G. Celeux, K. Lo and R. Gottardo (2010). Combining mixture components for clustering. *Journal of Computational and Graphical Statistics*, 19(2):332-353.

```
data(Baudry_etal_2010_JCGS_examples)
output <- clustCombi(ex4.1) # will run Mclust to get the MclustOutput
MclustOutput <- Mclust(ex4.1) # or you can run Mclust yourself
output <- clustCombi(ex4.1, MclustOutput) # and provide the output to clustCombi
# any further optional argument is passed to Mclust (see the Mclust documentation)
## Not run: output <- clustCombi(ex4.1, modelName = "EEV", G = 1:15)</pre>
output # is of class clustCombi
# plots the hierarchy of combined solutions, then some "entropy plots" which
# may help one to select the number of classes (please see the article cited
# in the references)
plot(output, ex4.1)
# the selected model and number of components by Mclust, ie by BIC with MLE
# on Gaussian mixtures
output$MclustOutput
# the selected number of components by Mclust: the combined hierarchy then
# starts from this number of classes and ends at one
output$MclustOutput$G
# the matrix whose [i,k]th entry is the probability that observation i in
```

20 combiPlot

```
# the data belongs to the kth class according to the BIC solution
head( output$combiz[[output$MclustOutput$G]] )
\# is the matrix whose [i,k]th entry is the probability that observation i in
# the data belongs to the kth class according to the first combined
# ((output$MclustOutput$G-1)-classes) solution
head( output$combiz[[output$MclustOutput$G-1]] )
# the matrix describing how to merge the 6-classes solution to get the
# 5-classes solution
output$combiM[[5]]
# for example the following code returns the label of the class (in the
# 5-classes combined solution) to which the 4th class (in the 6-classes
# solution) is assigned. Only two classes in the (K+1)-classes solution
# are assigned the same class in the K-classes solution: the two which
# are merged at this step...
output$combiM[[5]]
# recover the 5-classes soft clustering from the 6-classes soft clustering
# and the 6 -> 5 combining matrix
all( output$combiz[[5]] == t( output$combiM[[5]] %*% t(output$combiz[[6]]) ) )
# the hard clustering under the 5-classes solution
head( output$classification[[5]] )
```

combiPlot

Plot Classifications Corresponding to Successive Combined Solutions

Description

Plot classifications corresponding to successive combined solutions.

Usage

```
combiPlot(data, z, combiM, ...)
```

Arguments

data	The data.
Z	A matrix whose [i,k]th entry is the probability that observation i in the data belongs to the kth class, for the initial solution (ie before any combining). Typically, the one returned by Mclust/BIC.
combiM	A "combining matrix" (as provided by clustCombi), ie a matrix whose kth row contains only zeros, but in columns corresponding to the labels of the classes in the initial solution to be merged together to get the combined solution.
	Other arguments to be passed to the Mclust plot functions.

Value

Plot the classifications obtained by MAP from the matrix t(combiM %*% t(z)), which is the matrix whose [i,k]th entry is the probability that observation i in the data belongs to the kth class, according to the combined solution obtained by merging (according to combiM) the initial solution described by z.

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Author(s)

J.-P. Baudry, A. E. Raftery, L. Scrucca

References

J.-P. Baudry, A. E. Raftery, G. Celeux, K. Lo and R. Gottardo (2010). Combining mixture components for clustering. *Journal of Computational and Graphical Statistics*, 19(2):332-353.

See Also

```
clustCombi, combMat, clustCombi
```

Examples

```
data(Baudry_etal_2010_JCGS_examples)
MclustOutput <- Mclust(ex4.1)</pre>
MclustOutput$G # Mclust/BIC selected 6 classes
par(mfrow=c(2,2))
combiM0 = diag(6) # is the identity matrix
# no merging: plot the initial solution, given by z
combiPlot(ex4.1, MclustOutput$z, combiM0, cex = 3)
title("No combining")
combiM1 = combMat(6, 1, 2) # let's merge classes labeled 1 and 2
combiPlot(ex4.1, MclustOutput$z, combiM1)
title("Combine 1 and 2")
# let's merge classes labeled 1 and 2, and then components labeled (in this
# new 5-classes combined solution...) 1 and 2
combiM2 = combMat(5, 1, 2) %*% combMat(6, 1, 2)
combiM2
combiPlot(ex4.1, MclustOutput$z, combiM2)
title("Combine 1, 2 and then 1 and 2 again")
plot(0,0,type="n", xlab = "", ylab = "", axes = FALSE)
legend("center", legend = 1:6,
       col = mclust.options("classPlotColors"),
       pch = mclust.options("classPlotSymbols"),
       title = "Class labels:")
```

combMat

Combining Matrix

22 combMat

Description

Create a combining matrix

Usage

```
combMat(K, 11, 12)
```

Arguments

11

K	The original number of classes: the matrix will define a combining from K to
	(K-1) classes.

- Label of one of the two classes to be combined.
- Label of the other class to be combined.

Value

If z is a vector (length K) whose kth entry is the probability that an observation belongs to the kth class in a K-classes classification, then combiM %*% z is the vector (length K-I) whose kth entry is the probability that the observation belongs to the kth class in the K-I-classes classification obtained by merging classes 11 and 12 in the initial classification.

Author(s)

```
J.-P. Baudry, A. E. Raftery, L. Scrucca
```

References

J.-P. Baudry, A. E. Raftery, G. Celeux, K. Lo and R. Gottardo (2010). Combining mixture components for clustering. *Journal of Computational and Graphical Statistics*, 19(2):332-353.

See Also

```
clustCombi, combiPlot
```

Examples

```
\ensuremath{\text{\#}} Please see the documentation for the combiPlot function for an
```

illustration of how to use this function

23 coordProj

	coordProj	Coordinate projections of multidimensional data modeled by an MVN mixture.
--	-----------	--

Description

Plots coordinate projections given multidimensional data and parameters of an MVN mixture model for the data.

Usage

```
coordProj(data, dimens = c(1,2), parameters = NULL, z = NULL,
          classification = NULL, truth = NULL, uncertainty = NULL,
          what = c("classification", "errors", "uncertainty"),
          addEllipses = TRUE, symbols = NULL, colors = NULL, scale = FALSE,
          xlim = NULL, ylim = NULL, CEX = 1, PCH = ".", main = FALSE, ...)
```

data	A numeric matrix or data frame of observations. Categorical variables are not
	allowed. If a matrix or data frame, rows correspond to observations and columns
	correspond to variables.
dimens	A vector of length 2 giving the integer dimensions of the desired coordinate

projections. The default is c(1,2), in which the first dimension is plotted against the second.

A named list giving the parameters of an MCLUST model, used to produce superimposing ellipses on the plot. The relevant components are as follows:

mean The mean for each component. If there is more than one component, this is a matrix whose kth column is the mean of the kth component of the mixture model.

variance A list of variance parameters for the model. The components of this list depend on the model specification. See the help file for mclustVariance for details.

A matrix in which the [i,k]th entry gives the probability of observation i belonging to the kth class. Used to compute classification and uncertainty if those arguments aren't available.

classification A numeric or character vector representing a classification of observations (rows) of data. If present argument z will be ignored.

> A numeric or character vector giving a known classification of each data point. If classification or z is also present, this is used for displaying classification

> A numeric vector of values in (0,1) giving the uncertainty of each data point. If present argument z will be ignored.

> Choose from one of the following three options: "classification" (default), "errors", "uncertainty".

Arguments

parameters

z

truth

uncertainty

what

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addEllipses	A logical indicating whether or not to add ellipses with axes corresponding to the within-cluster covariances in case of "classification" or "uncertainty" plots.
symbols	Either an integer or character vector assigning a plotting symbol to each unique class in classification. Elements in colors correspond to classes in order of appearance in the sequence of observations (the order used by the function unique). The default is given by mclust.options("classPlotSymbols").
colors	Either an integer or character vector assigning a color to each unique class in classification. Elements in colors correspond to classes in order of appearance in the sequence of observations (the order used by the function unique). The default is given by mclust.options("classPlotColors").
scale	A logical variable indicating whether or not the two chosen dimensions should be plotted on the same scale, and thus preserve the shape of the distribution. Default: scale=FALSE
xlim, ylim	Arguments specifying bounds for the ordinate, abscissa of the plot. This may be useful for when comparing plots.
CEX	An argument specifying the size of the plotting symbols. The default value is 1.
PCH	An argument specifying the symbol to be used when a classification has not been specified for the data. The default value is a small dot ".".
main	A logical variable or NULL indicating whether or not to add a title to the plot identifying the dimensions used.
	Other graphics parameters.

Side Effects

A plot showing a two-dimensional coordinate projection of the data, together with the location of the mixture components, classification, uncertainty, and/or classification errors.

References

C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611-631*.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

```
{\tt clPairs, randProj, mclust2Dplot, mclust.options}
```

```
est <- meVVV(iris[,-5], unmap(iris[,5]))
## Not run:
par(pty = "s", mfrow = c(1,1))
coordProj(iris[,-5], dimens=c(2,3), parameters = est$parameters, z = est$z,</pre>
```

covw 25

COVW

Weighted means, covariance and scattering matrices conditioning on a weighted matrix.

Description

Compute efficiently (via Fortran code) the means, covariance and scattering matrices conditioning on a weighted or indicator matrix

Usage

```
covw(X, Z, normalize = TRUE)
```

Arguments

X A (nxp) data matrix, with n observations on p variables. Z A (nxG) matrix of weights, with G number of groups. A logical indicating if rows of Z should be normalized to sum to one.

Value

A list with the following components:

mean A(pxG) matrix of weighted means. S A(pxpxG) array of weighted covariance matrices. W A(pxpxG) array of weighted scattering matrices.

Author(s)

M. Fop and L. Scrucca

```
# Z as an indicator matrix
X = iris[,1:4]
Z = unmap(iris$Species)
str(covw(X, Z))
# Z as a matrix of weights
mod = Mclust(X, G = 3, modelNames = "VVV")
str(covw(X, mod$z))
```

26 cvMclustDA

cross

Simulated Cross Data

Description

A 500 by 3 matrix in which the first column is the classification and the remaining columns are two data from a simulation of two crossed elliptical Gaussians.

Usage

```
data(cross)
```

Examples

cvMclustDA

MclustDA cross-validation

Description

K-fold cross-validation for discriminant analysis based on Gaussian finite mixture modeling.

Usage

```
cvMclustDA(object, nfold = 10, verbose = TRUE, ...)
```

Arguments

object	An object of class 'MclustDA' resulting from a call to MclustDA.
nfold	An integer specifying the number of folds.
verbose	A logical, if TRUE and the session is interactive a text progress bar is displayed during the algorithm.
	Further arguments passed to or from other methods.

cvMclustDA 27

Value

The function returns a list with the following components:

classification a factor of cross-validated class labels.

error the cross-validation error.
se the standard error of cv error.

References

C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association* 97:611-631.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

Author(s)

Luca Scrucca

See Also

summary.MclustDA, plot.MclustDA, predict.MclustDA, classError

```
X <- iris[,-5]
Class <- iris[,5]

# common EEE covariance structure (which is essentially equivalent to linear discriminant analysis)
irisMclustDA <- MclustDA(X, Class, modelType = "EDDA", modelNames = "EEE")
cv <- cvMclustDA(irisMclustDA) # default 10-fold CV
cv[c("error", "se")]

cv <- cvMclustDA(irisMclustDA, nfold = length(Class)) # LOO-CV
cv[c("error", "se")]
# compare with
# cv1EMtrain(X, Class, "EEE")

# general covariance structure selected by BIC
irisMclustDA <- MclustDA(X, Class)
cv <- cvMclustDA(irisMclustDA) # default 10-fold CV
cv[c("error", "se")]</pre>
```

28 decomp2sigma

decomp2sigma	Convert mixture component covariances to matrix form.

Description

Converts covariances from a parameterization by eigenvalue decomposition or cholesky factorization to representation as a 3-D array.

Usage

```
decomp2sigma(d, G, scale, shape, orientation, ...)
```

Arguments

-	
d	The dimension of the data.
G	The number of components in the mixture model.
scale	Either a <i>G</i> -vector giving the scale of the covariance (the <i>d</i> th root of its determinant) for each component in the mixture model, or a single numeric value if the scale is the same for each component.
shape	Either a G by d matrix in which the k th column is the shape of the covariance matrix (normalized to have determinant 1) for the k th component, or a d -vector giving a common shape for all components.
orientation	Either a d by d by G array whose $[,,k]$ th entry is the orthonomal matrix whose columns are the eigenvectors of the covariance matrix of the k th component, or a d by d orthonormal matrix if the mixture components have a common orientation. The orientation component of decomp can be omitted in spherical and diagonal models, for which the principal components are parallel to the coordinate axes so that the orientation matrix is the identity.
	Catches unused arguments from an indirect or list call via do.call.

Value

A 3-D array whose [,,k]th component is the covariance matrix of the *k*th component in an MVN mixture model.

References

- C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611-631*.
- C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

sigma2decomp

defaultPrior 29

Examples

defaultPrior

Default conjugate prior for Gaussian mixtures.

Description

Default conjugate prior specification for Gaussian mixtures.

Usage

```
defaultPrior(data, G, modelName, ...)
```

Arguments

G

data

A numeric vector, matrix, or data frame of observations. Categorical variables are not allowed. If a matrix or data frame, rows correspond to observations and columns correspond to variables.

The number of mixture components.

modelName

A character string indicating the model:

"E": equal variance (univariate)

"V": variable variance (univariate)
"EII": spherical, equal volume

"VII": spherical, unequal volume

"EEI": diagonal, equal volume and shape

"VEI": diagonal, varying volume, equal shape

"EVI": diagonal, equal volume, varying shape

"" to the state of the state of

"VVI": diagonal, varying volume and shape

"EEE": ellipsoidal, equal volume, shape, and orientation

"EEV": ellipsoidal, equal volume and equal shape

"VEV": ellipsoidal, equal shape

"VVV": ellipsoidal, varying volume, shape, and orientation.

A description of the models above is provided in the help of mclustModelNames. Note that in the multivariate case only 10 out of 14 models may be used in conjunction with a prior, i.e. those available in *MCLUST* up to version 4.4.

30 defaultPrior

... One or more of the following:

dof The degrees of freedom for the prior on the variance. The default is d + 2, where d is the dimension of the data.

scale The scale parameter for the prior on the variance. The default is var(data)/G^(2/d), where d is the dimension of the data.

shrinkage The shrinkage parameter for the prior on the mean. The default value is 0.01. If 0 or NA, no prior is assumed for the mean.

mean The mean parameter for the prior. The default value is colMeans(data).

Details

defaultPrior is a function whose default is to output the default prior specification for EM within MCLUST.

Furthermore, defaultPrior can be used as a template to specify alternative parameters for a conjugate prior.

Value

A list giving the prior degrees of freedom, scale, shrinkage, and mean.

References

- C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611-631*.
- C. Fraley and A. E. Raftery (2005, revised 2009). Bayesian regularization for normal mixture estimation and model-based clustering. Technical Report, Department of Statistics, University of Washington.
- C. Fraley and A. E. Raftery (2007). Bayesian regularization for normal mixture estimation and model-based clustering. *Journal of Classification* 24:155-181.
- C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

```
mclustBIC, me, mstep, priorControl
```

dens 31

dens

Density for Parameterized MVN Mixtures

Description

Computes densities of observations in parameterized MVN mixtures.

Usage

```
dens(modelName, data, logarithm = FALSE, parameters, warn=NULL, ...)
```

Arguments

A numeric vector, matrix, or data frame of observations. Categorical variables are not allowed. If a matrix or data frame, rows correspond to observations and columns correspond to variables. A logical value indicating whether or not the logarithm of the component densities should be returned. The default is to return the component densities, obtained from the log component densities by exponentiation. parameters The parameters of the model: pro The vector of mixing proportions for the components of the mixture. mean The mean for each component. If there is more than one component, this is a matrix whose kth column is the mean of the kth component of the mixture model. variance A list of variance parameters for the model. The components of this list depend on the model specification. See the help file for mclustVariance for details. A logical value indicating whether or not a warning should be issued when computations fail. The default is warn=FALSE. Catches unused arguments in indirect or list calls via do. call.	modelName	A character string indicating the model. The help file for mclustModelNames describes the available models.
sities should be returned. The default is to return the component densities, obtained from the log component densities by exponentiation. The parameters of the model: pro The vector of mixing proportions for the components of the mixture. mean The mean for each component. If there is more than one component, this is a matrix whose kth column is the mean of the kth component of the mixture model. variance A list of variance parameters for the model. The components of this list depend on the model specification. See the help file for mclustVariance for details. warn A logical value indicating whether or not a warning should be issued when computations fail. The default is warn=FALSE.	data	are not allowed. If a matrix or data frame, rows correspond to observations and
pro The vector of mixing proportions for the components of the mixture. mean The mean for each component. If there is more than one component, this is a matrix whose kth column is the mean of the kth component of the mixture model. variance A list of variance parameters for the model. The components of this list depend on the model specification. See the help file for mclustVariance for details. A logical value indicating whether or not a warning should be issued when computations fail. The default is warn=FALSE.	logarithm	sities should be returned. The default is to return the component densities, ob-
mean The mean for each component. If there is more than one component, this is a matrix whose kth column is the mean of the kth component of the mixture model. variance A list of variance parameters for the model. The components of this list depend on the model specification. See the help file for mclustVariance for details. A logical value indicating whether or not a warning should be issued when computations fail. The default is warn=FALSE.	parameters	The parameters of the model:
this is a matrix whose kth column is the mean of the <i>k</i> th component of the mixture model. variance A list of variance parameters for the model. The components of this list depend on the model specification. See the help file for mclustVariance for details. Warn A logical value indicating whether or not a warning should be issued when computations fail. The default is warn=FALSE.		pro The vector of mixing proportions for the components of the mixture.
list depend on the model specification. See the help file for mclustVariance for details. Warn A logical value indicating whether or not a warning should be issued when computations fail. The default is warn=FALSE.		this is a matrix whose kth column is the mean of the kth component of the
putations fail. The default is warn=FALSE.		list depend on the model specification. See the help file for mclustVariance
Catches unused arguments in indirect or list calls via do.call.	warn	
•		Catches unused arguments in indirect or list calls via do.call.

Value

A numeric vector whose *i*th component is the density of the *ith* observation in data in the MVN mixture specified by parameters.

32 densityMclust

References

C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611-631*.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

```
cdens, mclust.options, do.call
```

Examples

densityMclust

Density Estimation via Model-Based Clustering

Description

Produces a density estimate for each data point using a Gaussian finite mixture model from Mclust.

Usage

```
densityMclust(data, ...)
```

Arguments

data

A numeric vector, matrix, or data frame of observations. Categorical variables are not allowed. If a matrix or data frame, rows correspond to observations and columns correspond to variables.

. . .

Additional arguments for the Mclust function. In particular, setting the arguments G and modelNames allow to specify the number of mixture components and the type of model to be fitted. By default an "optimal" model is selected based on the BIC criterion.

densityMclust 33

Value

An object of class densityMclust, which inherits from Mclust, is returned with the following slot added:

density The density evaluated at the input data computed from the estimated model.

References

C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611:631*.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

Author(s)

Revised version by Luca Scrucca based on the original code by C. Fraley and A.E. Raftery.

See Also

```
plot.densityMclust, Mclust, summary.Mclust, predict.densityMclust.
```

```
dens = densityMclust(faithful$waiting)
summary(dens)
summary(dens, parameters = TRUE)
plot(dens, what = "BIC", legendArgs = list(x = "topright"))
plot(dens, what = "density", data = faithful$waiting)
dens = densityMclust(faithful)
summary(dens)
summary(dens, parameters = TRUE)
plot(dens, what = "density", data = faithful)
plot(dens, what = "density", data = faithful,
     drawlabels = FALSE, points.pch = 20, col = "grey",
     levels = quantile(dens$density, probs = c(0.05, 0.25, 0.5, 0.75, 0.95)))
plot(dens, what = "density", type = "image", col = topo.colors(50))
plot(dens, what = "density", type = "persp")
dens = densityMclust(iris[,1:4])
summary(dens, parameters = TRUE)
plot(dens, what = "density", data = iris[,1:4],
     col = "slategrey", drawlabels = FALSE, nlevels = 7)
## Not run:
 plot(dens, what = "density", type = "image", col = "slategrey")
 plot(dens, what = "density", type = "persp", col = grey(0.9))
## End(Not run)
```

densityMclust.diagnostic

Diagnostic plots for mclustDensity estimation

Description

Diagnostic plots for density estimation. Only available for the one-dimensional case.

Usage

Arguments

object	An object of class 'mclustDensity' obtained from a call to densityMclust function.
type	The type of graph requested:
	"cdf" = a plot of the estimated CDF versus the empirical distribution function.
	"qq" = a Q-Q plot of sample quantiles versus the quantiles obtained from the inverse of the estimated cdf.
col	A pair of values for the color to be used for plotting, respectively, the estimated CDF and the empirical cdf.
lwd	A pair of values for the line width to be used for plotting, respectively, the estimated CDF and the empirical cdf.
lty	A pair of values for the line type to be used for plotting, respectively, the estimated CDF and the empirical cdf.
legend	A logical indicating if a legend must be added to the plot of fitted CDF vs the empirical CDF.
grid	A logical indicating if a grid should be added to the plot.
main	A logical indicating if a title should be added to the plot.
	Additional arguments.

Details

The two diagnostic plots for density estimation in the one-dimensional case are discussed in Loader (1999, pp- 87-90).

diabetes 35

References

Loader C. (1999), Local Regression and Likelihood. New York, Springer.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

Author(s)

Luca Scrucca

See Also

densityMclust, plot.densityMclust.

Examples

```
x = faithful$waiting
dens = densityMclust(x)
## Not run:
plot(dens, x, what = "diagnostic")
## End(Not run)
# or
densityMclust.diagnostic(dens, type = "cdf")
densityMclust.diagnostic(dens, type = "qq")
```

diabetes

Diabetes data

Description

The data set contains three measurements made on 145 non-obese adult patients classified into three groups.

Usage

```
data(diabetes)
```

Format

A data frame with the following variables:

class The type of diabete: Normal, Overt, and Chemical.

glucose Area under plasma glucose curve after a three hour oral glucose tolerance test (OGTT).

insulin Area under plasma insulin curve after a three hour oral glucose tolerance test (OGTT).

sspg Steady state plasma glucose.

36 em

Source

Reaven, G. M. and Miller, R. G. (1979). An attempt to define the nature of chemical diabetes using a multidimensional analysis. *Diabetologia* 16:17-24.

ture models.	em	EM algorithm starting with E-step for parameterized Gaussian mixture models.
--------------	----	--

Description

Implements the EM algorithm for parameterized Gaussian mixture models, starting with the expectation step.

Usage

```
em(modelName, data, parameters, prior = NULL, control = emControl(),
    warn = NULL, ...)
```

Arguments

modelName	A character string indicating the model.	The help file for mclustModelNames
	describes the available models.	

A numeric vector, matrix, or data frame of observations. Categorical variables are not allowed. If a matrix or data frame, rows correspond to observations and

columns correspond to variables.

A names list giving the parameters of the model. The components are as follows:

pro Mixing proportions for the components of the mixture. If the model includes a Poisson term for noise, there should be one more mixing proportion than the number of Gaussian components.

mean The mean for each component. If there is more than one component, this is a matrix whose kth column is the mean of the *k*th component of the mixture model.

variance A list of variance parameters for the model. The components of this list depend on the model specification. See the help file for mclustVariance for details.

Vinv An estimate of the reciprocal hypervolume of the data region. If set to NULL or a negative value, the default is determined by applying function hypvol to the data. Used only when pro includes an additional mixing proportion for a noise component.

Specification of a conjugate prior on the means and variances. The default assumes no prior.

A list of control parameters for EM. The defaults are set by the call emControl().

A logical value indicating whether or not a warning should be issued when computations fail. The default is warn=FALSE.

Catches unused arguments in indirect or list calls via do. call.

Arguments

data

parameters

prior

control

warn

. . .

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Value

A list including the following components:

modelName A character string identifying the model (same as the input argument).

n The number of observations in the data.

d The dimension of the data.

G The number of mixture components.

z A matrix whose [i,k]th entry is the conditional probability of the *i*th observa-

tion belonging to the kth component of the mixture.

parameters pro A vector whose kth component is the mixing proportion for the kth compo-

nent of the mixture model. If the model includes a Poisson term for noise, there should be one more mixing proportion than the number of Gaussian

components.

mean The mean for each component. If there is more than one component, this is a matrix whose kth column is the mean of the *k*th component of the

mixture model.

variance A list of variance parameters for the model. The components of this list depend on the model specification. See the help file for mclustVariance

for details.

Vinv The estimate of the reciprocal hypervolume of the data region used in the computation when the input indicates the addition of a noise component to

the model.

loglik The log likelihood for the data in the mixture model.

control The list of control parameters for EM used.

prior The specification of a conjugate prior on the means and variances used, NULL if

no prior is used.

Attributes: "info" Information on the iteration.

"WARNING" An appropriate warning if problems are encountered in the compu-

tations.

References

C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611-631*.

C. Fraley and A. E. Raftery (2005). Bayesian regularization for normal mixture estimation and model-based clustering. Technical Report, Department of Statistics, University of Washington.

C. Fraley and A. E. Raftery (2007). Bayesian regularization for normal mixture estimation and model-based clustering. *Journal of Classification* 24:155-181.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

 $\verb"emE", \dots, \verb"emVVV", estep, \verb"me", \verb"mstep", \verb"mclust.options", \verb"do.call"$

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Examples

emControl

Set control values for use with the EM algorithm.

Description

Supplies a list of values including tolerances for singularity and convergence assessment, for use functions involving EM within *MCLUST*.

Usage

```
emControl(eps, tol, itmax, equalPro)
```

Arguments

eps

A scalar tolerance associated with deciding when to terminate computations due to computational singularity in covariances. Smaller values of eps allow computations to proceed nearer to singularity. The default is the relative machine precision .Machine\$double.eps, which is approximately 2e-16 on IEEE-compliant machines.

tol

A vector of length two giving relative convergence tolerances for the log-likelihood and for parameter convergence in the inner loop for models with iterative M-step ("VEI", "EVE", "VEE", "VEV"), respectively. The default is c(1.e-5,sqrt(.Machine\$double.eps)). If only one number is supplied, it is used as the tolerance for the outer iterations and the tolerance for the inner iterations is as in the default.

itmax

A vector of length two giving integer limits on the number of EM iterations and on the number of iterations in the inner loop for models with iterative M-step ("VEI", "EVE", "VEE", "VVE", "VEV"), respectively. The default is c(.Machine\$integer.max, .Machine\$integer.max) allowing termination to be completely governed by tol. If only one number is supplied, it is used as the iteration limit for the outer iteration only.

equalPro

Logical variable indicating whether or not the mixing proportions are equal in the model. Default: equalPro = FALSE.

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Details

emControl is provided for assigning values and defaults for EM within MCLUST.

Value

A named list in which the names are the names of the arguments and the values are the values supplied to the arguments.

References

- C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611-631*.
- C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

```
em, estep, me, mstep, mclustBIC
```

Examples

```
irisBIC <- mclustBIC(iris[,-5], control = emControl(tol = 1.e-6))
summary(irisBIC, iris[,-5])</pre>
```

emE

EM algorithm starting with E-step for a parameterized Gaussian mixture model.

Description

Implements the EM algorithm for a parameterized Gaussian mixture model, starting with the expectation step.

Usage

```
emE(data, parameters, prior = NULL, control = emControl(), warn = NULL, ...)
emV(data, parameters, prior = NULL, control = emControl(), warn = NULL, ...)
emX(data, prior = NULL, warn = NULL, ...)
emEII(data, parameters, prior = NULL, control = emControl(), warn = NULL, ...)
emVII(data, parameters, prior = NULL, control = emControl(), warn = NULL, ...)
emEEI(data, parameters, prior = NULL, control = emControl(), warn = NULL, ...)
emVEI(data, parameters, prior = NULL, control = emControl(), warn = NULL, ...)
emEVI(data, parameters, prior = NULL, control = emControl(), warn = NULL, ...)
emVVI(data, parameters, prior = NULL, control = emControl(), warn = NULL, ...)
emEEE(data, parameters, prior = NULL, control = emControl(), warn = NULL, ...)
emEEV(data, parameters, prior = NULL, control = emControl(), warn = NULL, ...)
```

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```
emVEV(data, parameters, prior = NULL, control = emControl(), warn = NULL, ...)
emVVV(data, parameters, prior = NULL, control = emControl(), warn = NULL, ...)
emEVE(data, parameters, prior = NULL, control = emControl(), warn = NULL, ...)
emEVV(data, parameters, prior = NULL, control = emControl(), warn = NULL, ...)
emVEE(data, parameters, prior = NULL, control = emControl(), warn = NULL, ...)
emVVE(data, parameters, prior = NULL, control = emControl(), warn = NULL, ...)
emXXI(data, prior = NULL, warn = NULL, ...)
emXXX(data, prior = NULL, warn = NULL, ...)
```

Arguments

data

A numeric vector, matrix, or data frame of observations. Categorical variables are not allowed. If a matrix or data frame, rows correspond to observations and columns correspond to variables.

parameters

The parameters of the model:

pro Mixing proportions for the components of the mixture. There should one more mixing proportion than the number of Gaussian components if the mixture model includes a Poisson noise term.

mean The mean for each component. If there is more than one component, this is a matrix whose kth column is the mean of the *k*th component of the mixture model.

variance A list of variance parameters for the model. The components of this list depend on the model specification. See the help file for mclustVariance for details.

Vinv An estimate of the reciprocal hypervolume of the data region. The default is determined by applying function hypvol to the data. Used only when pro includes an additional mixing proportion for a noise component.

prior

The default assumes no prior, but this argument allows specification of a conjugate prior on the means and variances through the function priorControl.

control

A list of control parameters for EM. The defaults are set by the call emControl().

warn

A logical value indicating whether or not a warning should be issued whenever a singularity is encountered. The default is given in mclust.options("warn").

. . .

Catches unused arguments in indirect or list calls via do. call.

Value

A list including the following components:

modelName A characte

A character string identifying the model (same as the input argument).

z

A matrix whose [i,k]th entry is the conditional probability of the ith observation belonging to the kth component of the mixture.

parameters

pro A vector whose *k*th component is the mixing proportion for the *k*th component of the mixture model. If the model includes a Poisson term for noise, there should be one more mixing proportion than the number of Gaussian components.

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mean The mean for each component. If there is more than one component, this is a matrix whose kth column is the mean of the *k*th component of the mixture model.

variance A list of variance parameters for the model. The components of this list depend on the model specification. See the help file for mclustVariance for details.

Vinv The estimate of the reciprocal hypervolume of the data region used in the computation when the input indicates the addition of a noise component to the model.

loglik

The log likelihood for the data in the mixture model.

Attributes:

"info" Information on the iteration.

"WARNING" An appropriate warning if problems are encountered in the computations.

References

- C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association* 97:611-631.
- C. Fraley and A. E. Raftery (2005). Bayesian regularization for normal mixture estimation and model-based clustering. Technical Report, Department of Statistics, University of Washington.
- C. Fraley and A. E. Raftery (2007). Bayesian regularization for normal mixture estimation and model-based clustering. *Journal of Classification* 24:155-181.
- C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

```
me, mstep, mclustVariance, mclust.options.
```

Examples

```
msEst <- mstepEEE(data = iris[,-5], z = unmap(iris[,5]))
names(msEst)

emEEE(data = iris[,-5], parameters = msEst$parameters)</pre>
```

entPlot

Plot Entropy Plots

Description

Plot "entropy plots" to help select the number of classes from a hierarchy of combined clusterings.

Usage

```
entPlot(z, combiM, abc = c("standard", "normalized"), reg = 2, ...)
```

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Arguments

Z	A matrix whose $[i,k]$ th entry is the probability that observation i in the data belongs to the k th class, for the initial solution (ie before any combining). Typically, the one returned by Mclust/BIC.
combiM	A list of "combining matrices" (as provided by clustCombi), ie combiM[[K]] is the matrix whose k th row contains only zeros, but in columns corresponding to the labels of the classes in the $(K+1)$ -classes solution to be merged to get the K -classes combined solution. combiM must contain matrices from K = number of classes in z to one.
abc	Choose one or more of: "standard", "normalized", to specify whether the number of observations involved in each combining step should be taken into account to scale the plots or not.
reg	The number of parts of the piecewise linear regression for the entropy plots. Choose one or more of: 2 (for 1 change-point), 3 (for 2 change-points).
	Other graphical arguments to be passed to the plot functions.

Details

Please see the article cited in the references for more details. A clear elbow in the "entropy plot" should suggest the user to consider the corresponding number(s) of class(es).

Value

if abc = "standard", plots the entropy against the number of clusters and the difference between the entropy of successive combined solutions against the number of clusters. if abc = "normalized", plots the entropy against the cumulated number of observations involved in the successive combining steps and the difference between the entropy of successive combined solutions divided by the number of observations involved in the corresponding combining step against the number of clusters.

Author(s)

J.-P. Baudry, A. E. Raftery, L. Scrucca

References

J.-P. Baudry, A. E. Raftery, G. Celeux, K. Lo and R. Gottardo (2010). Combining mixture components for clustering. *Journal of Computational and Graphical Statistics*, 19(2):332-353.

See Also

```
plot.clustCombi, combiPlot, clustCombi
```

```
## Not run:
data(Baudry_etal_2010_JCGS_examples)
# run Mclust to get the MclustOutput
```

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```
output <- clustCombi(ex4.2, modelNames = "VII")
entPlot(output$MclustOutput$z, output$combiM, reg = c(2,3))
# legend: in red, the single-change-point piecewise linear regression;
# in blue, the two-change-point piecewise linear regression.
## End(Not run)</pre>
```

errorBars

Draw error bars on a plot

Description

Draw error bars at x from upper to lower. If horizontal = FALSE (default) bars are drawn vertically, otherwise horizontally.

Usage

```
errorBars(x, upper, lower, width = 0.1, code = 3, angle = 90, horizontal = FALSE, ...)
```

Arguments

Х	A vector of values where the bars must be drawn.
upper	A vector of upper values where the bars must end.
lower	A vector of lower values where the bars must start.
width	A value specifying the width of the end-point segment.
code	An integer code specifying the kind of arrows to be drawn. For details see arrows.
angle	A value specifying the angle at the arrow edge. For details see arrows.
horizontal	A logical specifying if bars should be drawn vertically (default) or horizontally.
	Further arguments are passed to arrows.

```
par(mfrow=c(2,2))
# Create a simple example dataset
x <- 1:5
n <- c(10, 15, 12, 6, 3)
se <- c(1, 1.2, 2, 1, .5)
# upper and lower bars
b <- barplot(n, ylim = c(0, max(n)*1.5))
errorBars(b, lower = n-se, upper = n+se, lwd = 2, col = "red3")
# one side bars
b <- barplot(n, ylim = c(0, max(n)*1.5))
errorBars(b, lower = n, upper = n+se, lwd = 2, col = "red3", code = 1)
# plot(x, n, ylim = c(0, max(n)*1.5), pch = 0)</pre>
```

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```
errorBars(x, lower = n-se, upper = n+se, lwd = 2, col = "red3")
dotchart(n, labels = x, pch = 19, xlim = c(0, max(n)*1.5))
errorBars(x, lower = n-se, upper = n+se, col = "red3", horizontal = TRUE)
```

estep

E-step for parameterized Gaussian mixture models.

Description

Implements the expectation step of EM algorithm for parameterized Gaussian mixture models.

Usage

```
estep( modelName, data, parameters, warn = NULL, ...)
```

Arguments

data

modelName A character string indicating the model. The help file for mclustModelNames

describes the available models.

A numeric vector, matrix, or data frame of observations. Categorical variables are not allowed. If a matrix or data frame, rows correspond to observations and

columns correspond to variables.

A names list giving the parameters of the model. The components are as follows: parameters

> pro Mixing proportions for the components of the mixture. If the model includes a Poisson term for noise, there should be one more mixing proportion than the number of Gaussian components.

> mean The mean for each component. If there is more than one component, this is a matrix whose kth column is the mean of the kth component of the mixture model.

> variance A list of variance parameters for the model. The components of this list depend on the model specification. See the help file for mclustVariance for details.

> Vinv An estimate of the reciprocal hypervolume of the data region. If set to NULL or a negative value, the default is determined by applying function hypvol to the data. Used only when pro includes an additional mixing proportion for a noise component.

A logical value indicating whether or not a warning should be issued when computations fail. The default is warn=FALSE.

Catches unused arguments in indirect or list calls via do. call.

warn

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Value

A list including the following components:

modelName A character string identifying the model (same as the input argument).

z A matrix whose [i,k]th entry is the conditional probability of the ith observa-

tion belonging to the kth component of the mixture.

parameters The input parameters.

loglik The log-likelihood for the data in the mixture model.

Attributes "WARNING": an appropriate warning if problems are encountered in the compu-

tations.

References

C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611-631*.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

```
estepE, ..., estepVVV, em, mstep, mclust.options mclustVariance
```

Examples

estepE

E-step in the EM algorithm for a parameterized Gaussian mixture model.

Description

Implements the expectation step in the EM algorithm for a parameterized Gaussian mixture model.

Usage

```
estepE(data, parameters, warn = NULL, ...)
estepV(data, parameters, warn = NULL, ...)
estepEII(data, parameters, warn = NULL, ...)
estepVII(data, parameters, warn = NULL, ...)
estepEEI(data, parameters, warn = NULL, ...)
```

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```
estepVEI(data, parameters, warn = NULL, ...)
estepEVI(data, parameters, warn = NULL, ...)
estepVVI(data, parameters, warn = NULL, ...)
estepEEE(data, parameters, warn = NULL, ...)
estepEEV(data, parameters, warn = NULL, ...)
estepVEV(data, parameters, warn = NULL, ...)
estepVVV(data, parameters, warn = NULL, ...)
estepEVE(data, parameters, warn = NULL, ...)
estepEVV(data, parameters, warn = NULL, ...)
estepVEE(data, parameters, warn = NULL, ...)
estepVVE(data, parameters, warn = NULL, ...)
```

Arguments

data

A numeric vector, matrix, or data frame of observations. Categorical variables are not allowed. If a matrix or data frame, rows correspond to observations and columns correspond to variables.

parameters

The parameters of the model:

pro Mixing proportions for the components of the mixture. If the model includes a Poisson term for noise, there should be one more mixing proportion than the number of Gaussian components.

mu The mean for each component. If there is more than one component, this is a matrix whose columns are the means of the components.

variance A list of variance parameters for the model. The components of this list depend on the model specification. See the help file for mclustVariance for details.

Vinv An estimate of the reciprocal hypervolume of the data region. If not supplied or set to a negative value, the default is determined by applying function hypvol to the data. Used only when pro includes an additional mixing proportion for a noise component.

warn

A logical value indicating whether or certain warnings should be issued. The default is given by mclust.options("warn").

• • •

Catches unused arguments in indirect or list calls via do. call.

Value

A list including the following components:

modelName Character string identifying the model.

z A matrix whose [i,k]th entry is the conditional probability of the *i*th observa-

tion belonging to the kth component of the mixture.

parameters The input parameters.

loglik The logliklihood for the data in the mixture model.

Attribute "WARNING": An appropriate warning if problems are encountered in the compu-

tations.

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References

C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association*.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

```
estep, em, mstep, do.call, mclustVariance, mclust.options.
```

Examples

```
msEst <- mstepEII(data = iris[,-5], z = unmap(iris[,5]))
names(msEst)
estepEII(data = iris[,-5], parameters = msEst$parameters)</pre>
```

GvHD

GvHD Dataset

Description

GvHD (Graft-versus-Host Disease) data of Brinkman et al. (2007). Two samples of this flow cytometry data, one from a patient with the GvHD, and the other from a control patient. The GvHD positive and control samples consist of 9083 and 6809 observations, respectively. Both samples include four biomarker variables, namely, CD4, CD8b, CD3, and CD8. The objective of the analysis is to identify CD3+ CD4+ CD8b+ cell sub-populations present in the GvHD positive sample.

A treatment of this data by combining mixtures is proposed in Baudry et al. (2010).

Usage

```
data(GvHD)
```

Format

GvHD.pos (positive patient) is a data frame with 9083 observations on the following 4 variables, which are biomarker measurements.

CD4

CD8b

CD3

CD8

GvHD.control (control patient) is a data frame with 6809 observations on the following 4 variables, which are biomarker measurements.

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CD4

CD8b

CD3

CD8

References

R. R. Brinkman, M. Gasparetto, S.-J. J. Lee, A. J. Ribickas, J. Perkins, W. Janssen, R. Smiley and C. Smith (2007). High-content flow cytometry and temporal data analysis for defining a cellular signature of Graft-versus-Host Disease. *Biology of Blood and Marrow Transplantation*, 13: 691-700.

K. Lo, R. R. Brinkman, R. Gottardo (2008). Automated gating of flow cytometry data via robust model-based clustering. *Cytometry A*, 73: 321-332.

J.-P. Baudry, A. E. Raftery, G. Celeux, K. Lo and R. Gottardo (2010). Combining mixture components for clustering. *Journal of Computational and Graphical Statistics*, 19(2):332-353.

Examples

```
## Not run:
data(GvHD)

dat <- GvHD.pos[1:500,] # only a few lines for a quick example

output <- clustCombi(dat)

output # is of class clustCombi

# plots the hierarchy of combined solutions, then some "entropy plots" which
# may help one to select the number of classes
plot(output, dat)

## End(Not run)</pre>
```

hc

Model-based Hierarchical Clustering

Description

Agglomerative hierarchical clustering based on maximum likelihood criteria for Gaussian mixture models parameterized by eigenvalue decomposition.

Usage

```
hc(data,
  modelName = mclust.options("hcModelNames")[1],
  use = mclust.options("hcUse"), ...)
```

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Arguments

data A numeric vector, matrix, or data frame of observations. Categorical variables

are not allowed. If a matrix or data frame, rows correspond to observations and

columns correspond to variables.

modelName A character string indicating the model to be used.

Possible models are:

"E": equal variance (one-dimensional)

"V": spherical, variable variance (one-dimensional)

"EII": spherical, equal volume
"VII": spherical, unequal volume

"EEE": ellipsoidal, equal volume, shape, and orientation "VVV": ellipsoidal, varying volume, shape, and orientation.

By default the first model listed in mclust.options("hcModelNames"), i.e.

"VVV", is used.

A character string specifying what type of data/transformation should be used

for model-based hierarchical clustering.

This is experimental and it is only useful for the initialization of EM algorithm. By default it uses the method specified in mclust.options("hcUse"), which

is set to "VARS", i.e. the original input variables.

... Arguments for the method-specific hc functions. See for example hcE.

Details

Most models have memory usage of the order of the square of the number groups in the initial partition for fast execution. Some models, such as equal variance or "EEE", do not admit a fast algorithm under the usual agglomerative hierarchical clustering paradigm. These use less memory but are much slower to execute.

Value

A numeric two-column matrix in which the *i*th row gives the minimum index for observations in each of the two clusters merged at the *i*th stage of agglomerative hierarchical clustering.

References

- J. D. Banfield and A. E. Raftery (1993). Model-based Gaussian and non-Gaussian Clustering. *Biometrics* 49:803-821.
- C. Fraley (1998). Algorithms for model-based Gaussian hierarchical clustering. *SIAM Journal on Scientific Computing* 20:270-281.
- C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611-631*.
- C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

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Note

If modelName = "E" (univariate with equal variances) or modelName = "EII" (multivariate with equal spherical covariances), then the method is equivalent to Ward's method for hierarchical clustering.

See Also

```
hcE,..., hcVVV, hclass, mclust.options
```

Examples

```
hcTree <- hc(modelName = "VVV", data = iris[,-5])
cl <- hclass(hcTree,c(2,3))

## Not run:
par(pty = "s", mfrow = c(1,1))
clPairs(iris[,-5],cl=cl[,"2"])
clPairs(iris[,-5],cl=cl[,"3"])

par(mfrow = c(1,2))
dimens <- c(1,2)
coordProj(iris[,-5], dimens = dimens, classification=cl[,"2"])
coordProj(iris[,-5], dimens = dimens, classification=cl[,"3"])

## End(Not run)</pre>
```

hcE

Model-based Hierarchical Clustering

Description

Agglomerative hierarchical clustering based on maximum likelihood for a Gaussian mixture model parameterized by eigenvalue decomposition.

Usage

```
hcE(data, partition, minclus=1, ...)
hcV(data, partition, minclus = 1, alpha = 1, ...)
hcEII(data, partition, minclus = 1, ...)
hcVII(data, partition, minclus = 1, alpha = 1, ...)
hcEEE(data, partition, minclus = 1, ...)
hcVVV(data, partition, minclus = 1, alpha = 1, beta = 1, ...)
```

Arguments

data

A numeric vector, matrix, or data frame of observations. Categorical variables are not allowed. If a matrix or data frame, rows correspond to observations and columns correspond to variables.

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partition	A numeric or character vector representing a partition of observations (rows) of data. If provided, group merges will start with this partition. Otherwise, each observation is assumed to be in a cluster by itself at the start of agglomeration.
minclus	A number indicating the number of clusters at which to stop the agglomeration. The default is to stop when all observations have been merged into a single cluster.
alpha, beta	Additional tuning parameters needed for initialization in some models. For details, see Fraley 1998. The defaults provided are usually adequate.
	Catch unused arguments from a do.call call.

Details

Most models have memory usage of the order of the square of the number groups in the initial partition for fast execution. Some models, such as equal variance or "EEE", do not admit a fast algorithm under the usual agglomerative hierarchical clustering paradigm. These use less memory but are much slower to execute.

Value

A numeric two-column matrix in which the *i*th row gives the minimum index for observations in each of the two clusters merged at the *i*th stage of agglomerative hierarchical clustering.

References

- J. D. Banfield and A. E. Raftery (1993). Model-based Gaussian and non-Gaussian Clustering. *Biometrics* 49:803-821.
- C. Fraley (1998). Algorithms for model-based Gaussian hierarchical clustering. *SIAM Journal on Scientific Computing* 20:270-281.
- C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611-631*.
- C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

hc, hclass randomPairs

```
hcTree <- hcEII(data = iris[,-5])
cl <- hclass(hcTree,c(2,3))

## Not run:
par(pty = "s", mfrow = c(1,1))
clPairs(iris[,-5],cl=cl[,"2"])
clPairs(iris[,-5],cl=cl[,"3"])</pre>
```

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```
par(mfrow = c(1,2))
dimens <- c(1,2)
coordProj(iris[,-5], classification=cl[,"2"], dimens=dimens)
coordProj(iris[,-5], classification=cl[,"3"], dimens=dimens)
## End(Not run)</pre>
```

hclass

Classifications from Hierarchical Agglomeration

Description

Determines the classifications corresponding to different numbers of groups given merge pairs from hierarchical agglomeration.

Usage

```
hclass(hcPairs, G)
```

Arguments

hcPairs	A numeric two-column matrix in which the <i>i</i> th row gives the minimum index for observations in each of the two clusters merged at the <i>i</i> th stage of agglomerative hierarchical clustering.
G	An integer or vector of integers giving the number of clusters for which the

corresponding classfications are wanted.

Value

A matrix with length(G) columns, each column corresponding to a classification. Columns are indexed by the character representation of the integers in G.

References

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

```
hc, hcE
```

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Examples

```
hcTree <- hc(modelName="VVV", data = iris[,-5])
cl <- hclass(hcTree,c(2,3))

## Not run:
par(pty = "s", mfrow = c(1,1))
clPairs(iris[,-5],cl=cl[,"2"])
clPairs(iris[,-5],cl=cl[,"3"])

## End(Not run)</pre>
```

hypvol

Aproximate Hypervolume for Multivariate Data

Description

Computes a simple approximation to the hypervolume of a multivariate data set.

Usage

```
hypvol(data, reciprocal=FALSE)
```

Arguments

data

A numeric vector, matrix, or data frame of observations. Categorical variables are not allowed. If a matrix or data frame, rows correspond to observations and columns correspond to variables.

reciprocal

A logical variable indicating whether or not the reciprocal hypervolume is desired rather than the hypervolume itself. The default is to return the hypervolume.

Value

Returns the minimum of the hypervolume computed from simple variable bounds and that computed from variable bounds of the principal component scores. Used for the default hypervolume parameter for the noise component when observations are designated as noise in Mclust and mclustBIC.

References

- A. Dasgupta and A. E. Raftery (1998). Detecting features in spatial point processes with clutter via model-based clustering. *Journal of the American Statistical Association 93:294-302*.
- C. Fraley and A.E. Raftery (1998). Computer Journal 41:578-588.
- C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611-631*.

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See Also

```
mclustBIC
```

Examples

```
hypvol(iris[,-5])
```

icl

ICL for an estimated Gaussian Mixture Model

Description

Computes the ICL (Integrated Complete-data Likelihood) for criterion for a Gaussian Mixture Model fitted by Mclust.

Usage

```
icl(object, ...)
```

Arguments

object An object of class 'Mclust' resulting from a call to Mclust.
... Further arguments passed to or from other methods.

Value

The ICL for the given input MCLUST model.

References

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

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

```
Mclust, mclustBIC, mclustICL, bic.
```

```
mod = Mclust(iris[,1:4])
icl(mod)
```

imputeData 55

imputeData Missing Data Imputation via the mix package	
---	--

Description

Imputes missing data using the mix package.

Usage

```
imputeData(x, categorical = NULL, seed = NULL)
```

Arguments

Х	A numeric vector, matrix, or data frame of observations containing missing values. Categorical variables are allowed. If a matrix or data frame, rows correspond to observations and columns correspond to variables.
categorical	A logical vectors whose <i>i</i> th entry is TRUE if the <i>i</i> th variable or column of x is to be interpreted as categorical and FALSE otherwise. The default is to assume that a variable is to be interpreted as categorical only if it is a factor.
seed	A seed for the function rngseed that is used to initialize the random num-

A seed for the function rngseed that is used to initialize the random number generator in **mix**. By default, a seed is chosen uniformly in the interval (.Machine\$integer.max/1024, .Machine\$integer.max).

Value

A dataset of the same dimensions as x with missing values filled in.

References

J. L. Schafer, Analysis of Imcomplete Multivariate Data, Chapman and Hall, 1997.

See Also

```
imputePairs
```

```
# Note that package 'mix' must be installed.
## Not run:

# impute the continuos variables in the stlouis data
stlimp <- imputeData(stlouis[,-(1:3)])

# plot imputed values
imputePairs(stlouis[,-(1:3)], stlimp)

## End(Not run)</pre>
```

imputePairs

imputePairs	Pairwise Scatter Plots showing Missing Data Imputations

Description

Creates a scatter plot for each pair of variables in given data, allowing display of imputations for missing values in different colors and symbols than non missing values.

Usage

```
imputePairs(x, impx, symbols = c(16,1), colors = c("black", "red"), labels,
    panel = points, ..., lower.panel = panel, upper.panel = panel,
    diag.panel = NULL, text.panel = textPanel, label.pos = 0.5 +
    has.diag/3, cex.labels = NULL, font.labels = 1, row1attop = TRUE,
    gap = 0.2)
```

Arguments

x	A numeric vector, matrix, or data frame of observations containing missing values. Categorical variables are not allowed. If a matrix or data frame, rows correspond to observations and columns correspond to variables.
impx	The dataset x with missing values imputed.
symbols	Either an integer or character vector assigning plotting symbols to the nonmissing data and impued values, respectively. The default is a closed circle for the nonmissing data and an open circle for the imputed values.
colors	Either an integer or character vector assigning colors to the nonmissing data and impued values, respectively. The default is black for the nonmissing data and red for the imputed values.
labels	As in function pairs.
panel	As in function pairs.
• • •	As in function pairs.
lower.panel	As in function pairs.
upper.panel	As in function pairs.
diag.panel	As in function pairs.
text.panel	As in function pairs.
label.pos	As in function pairs.
cex.labels	As in function pairs.
font.labels	As in function pairs.
row1attop	As in function pairs.
gap	As in function pairs.

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Side Effects

A pairs plot displaying the location of missing and nonmissing values.

References

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

```
pairs, imputeData
```

Examples

```
# Note that package 'mix' must be installed.

# impute the continuos variables in the stlouis data
stlimp <- imputeData(stlouis[,-(1:3)])

# plot imputed values
imputePairs(stlouis[,-(1:3)], stlimp)</pre>
```

logLik.Mclust

Log-Likelihood of a Mclust object

Description

Returns the log-likelihood for a 'Mclust' object.

Usage

```
## S3 method for class 'Mclust'
logLik(object, ...)
```

Arguments

```
object an object of class 'Mclust' resulting from a call to Mclust.
... further arguments passed to or from other methods.
```

Value

Returns an object of class 'logLik' with an element providing the maximized log-likelihood, and further arguments giving the number of (estimated) parameters in the model ("df") and the sample size ("nobs").

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Author(s)

Luca Scrucca

References

C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611:631*.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

Mclust.

Examples

```
## Not run:
irisMclust <- Mclust(iris[,1:4])
summary(irisMclust)
logLik(irisMclust)
## End(Not run)</pre>
```

logLik.MclustDA

Log-Likelihood of a MclustDA object

Description

Returns the log-likelihood for a MclustDA object.

Usage

```
## S3 method for class 'MclustDA'
logLik(object, data, ...)
```

Arguments

object an object of class 'MclustDA' resulting from a call to MclustDA.

data the data for which the log-likelihood must be computed. If missing, the observed

data from the 'MclustDA' object is used.

... further arguments passed to or from other methods.

Value

Returns an object of class 'logLik' with an element providing the maximized log-likelihood, and further arguments giving the number of (estimated) parameters in the model ("df") and the sample size ("nobs").

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Author(s)

Luca Scrucca

References

C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611:631*.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

MclustDA.

Examples

```
## Not run:
irisMclustDA <- MclustDA(iris[,1:4], iris$Species)
summary(irisMclustDA)
logLik(irisMclustDA)
## End(Not run)</pre>
```

map

Classification given Probabilities

Description

Converts a matrix in which each row sums to I into the nearest matrix of (0,1) indicator variables.

Usage

```
map(z, warn = mclust.options("warn"), ...)
```

Arguments

Z	A matrix (for example a matrix of conditional probabilities in which each row sums to 1 as produced by the E-step of the EM algorithm).
warn	A logical variable indicating whether or not a warning should be issued when there are some columns of z for which no row attains a maximum.
	Provided to allow lists with elements other than the arguments can be passed in indirect or list calls with do call.

Value

A integer vector with one entry for each row of z, in which the *i*-th value is the column index at which the *i*-th row of z attains a maximum.

60 mapClass

References

C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611-631*.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

```
unmap, estep, em, me.
```

Examples

```
emEst <- me(modelName = "VVV", data = iris[,-5], z = unmap(iris[,5]))
map(emEst$z)</pre>
```

mapClass

Correspondence between classifications.

Description

Best correspondence between classes given two vectors viewed as alternative classifications of the same object.

Usage

```
mapClass(a, b)
```

Arguments

- a A numeric or character vector of class labels.
- b A numeric or character vector of class labels. Must have the same length as a.

Value

A list with two named elements, aTOb and bTOa which are themselves lists. The aTOb list has a component corresponding to each unique element of a, which gives the element or elements of b that result in the closest class correspondence.

The bT0a list has a component corresponding to each unique element of b, which gives the element or elements of a that result in the closest class correspondence.

See Also

```
mapClass, classError, table
```

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Examples

```
a <- rep(1:3, 3)
a
b <- rep(c("A", "B", "C"), 3)
b
mapClass(a, b)
a <- sample(1:3, 9, replace = TRUE)
a
b <- sample(c("A", "B", "C"), 9, replace = TRUE)
b
mapClass(a, b)</pre>
```

Mclust

Model-Based Clustering

Description

The optimal model according to BIC for EM initialized by hierarchical clustering for parameterized Gaussian mixture models.

Usage

```
Mclust(data, G = NULL, modelNames = NULL,
    prior = NULL,
    control = emControl(),
    initialization = NULL,
    warn = mclust.options("warn"),
    x = NULL, ...)
```

Arguments

data A numeric vector, matrix, or data frame of observations. Categorical variables

are not allowed. If a matrix or data frame, rows correspond to observations and

columns correspond to variables.

G An integer vector specifying the numbers of mixture components (clusters) for

which the BIC is to be calculated. The default is G=1:9.

modelNames A vector of character strings indicating the models to be fitted in the EM phase

of clustering. The default is:

```
for univariate data c("E", "V") for multivariate data (n > d) mclust.options("emModelNames") for multivariate data (n <= d) the spherical and diagonal models c("EII", "VII", "EEI", "EVI", "VVI")
```

The help file for mclustModelNames describes the available models.

prior The default assumes no prior, but this argument allows specification of a conju-

gate prior on the means and variances through the function priorControl.

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Note that, as described in defaultPrior, in the multivariate case only 10 out of 14 models may be used in conjunction with a prior, i.e. those available in *MCLUST* up to version 4.4.

control A list of control parameters for EM. The defaults are set by the call emControl().

initialization A list containing zero or more of the following components:

hcPairs A matrix of merge pairs for hierarchical clustering such as produced by function hc. For multivariate data, the default is to compute a hierarchical clustering tree by applying function hc with modelName = "VVV" to the data or a subset as indicated by the subset argument. The hierarchical clustering results are to start EM. For univariate data, the default is to use quantiles to start EM.

subset A logical or numeric vector specifying a subset of the data to be used in the initial hierarchical clustering phase.

noise A logical or numeric vector indicating an initial guess as to which observations are noise in the data. If numeric the entries should correspond to row indexes of the data. If supplied, a noise term will be added to the model in the estimation.

warn A logical value indicating whether or not certain warnings (usually related to

singularity) should be issued. The default is controlled by mclust.options.

An object of class 'mclustBIC'. If supplied, BIC values for models that have already been computed and are available in x are not recomputed. All arguments, with the exception of data, G and modelName, are ignored and their values are set as specified in the attributes of x. Defaults for G and modelNames are taken

from x.

... Catches unused arguments in indirect or list calls via do.call.

Value

Х

An object of class 'Mclust' providing the optimal (according to BIC) mixture model estimation.

The details of the output components are as follows:

call The matched call data The input data matrix.

modelName A character string denoting the model at which the optimal BIC occurs.

n The number of observations in the data.

d The dimension of the data.

G The optimal number of mixture components.

BIC All BIC values.
bic Optimal BIC value.

loglik The log-likelihood corresponding to the optimal BIC.

df The number of estimated parameters.

hypvol The hypervolume parameter for the noise component if required, otherwise set

to NULL (see hypvol).

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parameters

A list with the following components:

pro A vector whose *k*th component is the mixing proportion for the *k*th component of the mixture model. If missing, equal proportions are assumed.

mean The mean for each component. If there is more than one component, this is a matrix whose kth column is the mean of the *k*th component of the mixture model.

variance A list of variance parameters for the model. The components of this list depend on the model specification. See the help file for mclustVariance for details.

Z

A matrix whose [i,k]th entry is the probability that observation i in the test data belongs to the kth class.

classification The classification corresponding to z, i.e. map(z).
uncertainty The uncertainty associated with the classification.

References

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611:631*.

C. Fraley and A. E. Raftery (2005, revised 2009). Bayesian regularization for normal mixture estimation and model-based clustering. Technical Report, Department of Statistics, University of Washington.

C. Fraley and A. E. Raftery (2007). Bayesian regularization for normal mixture estimation and model-based clustering. *Journal of Classification* 24:155-181.

See Also

 $summary. \\ Mclust, plot. \\ Mclust, priorControl, emControl, hc, mclust BIC, mclust \\ Model \\ Names, mclust. \\ options$

```
mod1 = Mclust(iris[,1:4])
summary(mod1)

mod2 = Mclust(iris[,1:4], G = 3)
summary(mod2, parameters = TRUE)

# Using prior
mod3 = Mclust(iris[,1:4], prior = priorControl())
summary(mod3)

mod4 = Mclust(iris[,1:4], prior = priorControl(functionName="defaultPrior", shrinkage=0.1))
summary(mod4)

# Clustering of faithful data with some artificial noise added
```

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mclust-deprecated

Deprecated Functions in mclust package

Description

These functions are provided for compatibility with older versions of the **mclust** package only, and may be removed eventually.

Usage

```
cv.MclustDA(...)
cv1EMtrain(data, labels, modelNames=NULL)
bicEMtrain(data, labels, modelNames=NULL)
```

Arguments

... pass arguments down.

data A numeric vector or matrix of observations.

labels Labels for each element or row in the dataset.

modelNames Vector of model names that should be tested. The default is to select all available

model names.

mclust.options

Default values for use with MCLUST package

Description

Set or retrieve default values for use with MCLUST package.

Usage

```
mclust.options(...)
```

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Arguments

... one or more arguments provided in the name = value form, or no argument at all may be given.

Available arguments are described in the Details section below.

Details

mclust.options is provided for assigning values to the .mclust variable list, which is used to supply default values to various functions in MCLUST.

Available options are:

emModelNames A vector of 3-character strings that are associated with multivariate models for which EM estimation is available in MCLUST.

The current default is all of the multivariate mixture models supported in MCLUST. The help file for mclustModelNames describes the available models.

hcModelNames A vector of character strings associated with multivariate models for which model-based hierarchical clustering is available in MCLUST.

The available models are the following:

"EII" = spherical, equal volume

"EEE" = ellipsoidal, equal volume, shape, and orientation

"VII" = spherical, unequal volume

"VVV" = ellipsoidal, varying volume, shape, and orientation.

The last model in this list is used as default for initialization of EM-algorithm.

hcUse A string specifying the type of input variables to be used for model-based hierarchical clustering to start the EM-algorithm. Possible values are:

"VARS" = original variables (default);

"STD" = standardized variables;

"SPH" = sphered variables (centered, scaled, uncorrelated) computed using SVD;

"PCS" = principal components computed using SVD on centered variables (i.e. using the covariance matrix);

"PCR" = principal components computed using SVD on standardized (center and scaled) variables (i.e. using the correlation matrix);

"SVD" = scaled SVD transformation.

- bicPlotSymbols A vector whose entries correspond to graphics symbols for plotting the BIC values output from Mclust and mclustBIC. These are displayed in the legend which appears at the lower right of the BIC plots.
- bicPlotColors A vector whose entries correspond to colors for plotting the BIC curves from output from Mclust and mclustBIC. These are displayed in the legend which appears at the lower right of the BIC plots.
- classPlotSymbols A vector whose entries are either integers corresponding to graphics symbols or single characters for indicating classifications when plotting data. Classes are assigned symbols in the given order.
- classPlotColors A vector whose entries correspond to colors for indicating classifications when plotting data. Classes are assigned colors in the given order.
- warn A logical value indicating whether or not to issue certain warnings. Most of these warnings have to do with situations in which singularities are encountered. The default is warn = FALSE.

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The parameter values set via a call to this function will remain in effect for the rest of the session, affecting the subsequent behaviour of the functions for which the given parameters are relevant.

Value

If the argument list is empty the function returns the current list of values. If the argument list is not empty, the returned list is invisible.

References

C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611-631*.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

Mclust, MclustDA, densityMclust, emControl

```
opt <- mclust.options() # save default values</pre>
irisBIC <- mclustBIC(iris[,-5])</pre>
summary(irisBIC, iris[,-5])
mclust.options(emModelNames = c("EII", "EEI", "EEE"))
irisBIC <- mclustBIC(iris[,-5])</pre>
summary(irisBIC, iris[,-5])
mclust.options(opt)
                     # restore default values
mclust.options()
oldpar <- par(mfrow = c(2,1), no.readonly = TRUE)
n <- with(mclust.options(),</pre>
          max(sapply(list(bicPlotSymbols, bicPlotColors),length)))
plot(seq(n), rep(1,n), ylab = "", xlab = "", yaxt = "n",
     pch = mclust.options("bicPlotSymbols"),
     col = mclust.options("bicPlotColors"))
title("mclust.options(\"bicPlotSymbols\") \n mclust.options(\"bicPlotColors\")")
n <- with(mclust.options(),</pre>
          max(sapply(list(classPlotSymbols, classPlotColors),length)))
plot(seq(n), rep(1,n), ylab = "", xlab = "", yaxt = "n",
     pch = mclust.options("classPlotSymbols"),
     col = mclust.options("classPlotColors"))
title("mclust.options(\"classPlotSymbols\") \n mclust.options(\"classPlotColors\")")
par(oldpar)
```

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mclust1Dplot	Plot one-dimensional data modeled by an MVN mixture.	

Description

Plot one-dimensional data given parameters of an MVN mixture model for the data.

Usage

```
mclust1Dplot(data, parameters = NULL, z = NULL,
             classification = NULL, truth = NULL, uncertainty = NULL,
             what = c("classification", "density", "errors", "uncertainty"),
             symbols = NULL, colors = NULL, ngrid = length(data),
             xlab = NULL, xlim = NULL, CEX = 1,
             main = FALSE, ...)
```

Arguments

data A numeric vector of observations. Categorical variables are not allowed.

A named list giving the parameters of an MCLUST model, used to produce superimposing ellipses on the plot. The relevant components are as follows:

pro Mixing proportions for the components of the mixture. There should one more mixing proportion than the number of Gaussian components if the mixture model includes a Poisson noise term.

mean The mean for each component. If there is more than one component, this is a matrix whose kth column is the mean of the kth component of the mixture model.

variance A list of variance parameters for the model. The components of this list depend on the model specification. See the help file for mclustVariance for details.

A matrix in which the [i,k]th entry gives the probability of observation i belonging to the kth class. Used to compute classification and uncertainty if those arguments aren't available.

classification A numeric or character vector representing a classification of observations (rows) of data. If present argument z will be ignored.

> A numeric or character vector giving a known classification of each data point. If classification or z is also present, this is used for displaying classification errors.

> A numeric vector of values in (0,1) giving the uncertainty of each data point. If present argument z will be ignored.

> Choose from one of the following three options: "classification" (default), "density", "errors", "uncertainty".

parameters

z

truth

uncertainty

what

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symbols	Either an integer or character vector assigning a plotting symbol to each unique class classification. Elements in symbols correspond to classes in classification in order of appearance in the observations (the order used by the function unique). The default is to use a single plotting symbol . Classes are delineated by showing them in separate lines above the whole of the data.
colors	Either an integer or character vector assigning a color to each unique class classification. Elements in colors correspond to classes in order of appearance in the observations (the order used by the function unique). The default is given is mclust.options("classPlotColors").
ngrid	Number of grid points to use for density computation over the interval spanned by the data. The default is the length of the data set.
xlab	An argument specifying a label for the horizontal axis.
xlim	An argument specifying bounds of the plot. This may be useful for when comparing plots.
CEX	An argument specifying the size of the plotting symbols. The default value is 1.
main	A logical variable or NULL indicating whether or not to add a title to the plot identifying the dimensions used.
	Other graphics parameters.

Side Effects

A plot showing location of the mixture components, classification, uncertainty, density and/or classification errors. Points in the different classes are shown in separated levels above the whole of the data.

References

- C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611-631*.
- C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

```
mclust2Dplot, clPairs, coordProj
```

mclust2Dplot 69

mclust2Dplot

Plot two-dimensional data modelled by an MVN mixture.

Description

Plot two-dimensional data given parameters of an MVN mixture model for the data.

Usage

Arguments

data

A numeric matrix or data frame of observations. Categorical variables are not allowed. If a matrix or data frame, rows correspond to observations and columns correspond to variables. In this case the data are two dimensional, so there are two columns.

parameters

A named list giving the parameters of an *MCLUST* model, used to produce superimposing ellipses on the plot. The relevant components are as follows:

- pro Mixing proportions for the components of the mixture. There should one more mixing proportion than the number of Gaussian components if the mixture model includes a Poisson noise term.
- mean The mean for each component. If there is more than one component, this is a matrix whose kth column is the mean of the *k*th component of the mixture model.
- variance A list of variance parameters for the model. The components of this list depend on the model specification. See the help file for mclustVariance for details.

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Z	A matrix in which the $[i,k]$ th entry gives the probability of observation i belonging to the k th class. Used to compute classification and uncertainty if those arguments aren't available.
classification	A numeric or character vector representing a classification of observations (rows) of data. If present argument z will be ignored.
truth	A numeric or character vector giving a known classification of each data point. If classification or z is also present, this is used for displaying classification errors.
uncertainty	A numeric vector of values in $(0,1)$ giving the uncertainty of each data point. If present argument z will be ignored.
what	Choose from one of the following three options: "classification" (default), "errors", "uncertainty".
addEllipses	A logical indicating whether or not to add ellipses with axes corresponding to the within-cluster covariances.
symbols	Either an integer or character vector assigning a plotting symbol to each unique class in classification. Elements in colors correspond to classes in order of appearance in the sequence of observations (the order used by the function unique). The default is given by mclust.options("classPlotSymbols").
colors	Either an integer or character vector assigning a color to each unique class in classification. Elements in colors correspond to classes in order of appearance in the sequence of observations (the order used by the function unique). The default is given is mclust.options("classPlotColors").
xlim, ylim	Optional argument specifying bounds for the ordinate, abscissa of the plot. This may be useful for when comparing plots.
xlab, ylab	Optional argument specifying labels for the x-axis and y-axis.
scale	A logical variable indicating whether or not the two chosen dimensions should be plotted on the same scale, and thus preserve the shape of the distribution. Default: scale=FALSE
CEX	An argument specifying the size of the plotting symbols. The default value is 1.
PCH	An argument specifying the symbol to be used when a classification has not been specified for the data. The default value is a small dot ".".
main	A logical variable or NULL indicating whether or not to add a title to the plot identifying the dimensions used.
swapAxes	A logical variable indicating whether or not the axes should be swapped for the plot.
	Other graphics parameters.

Side Effects

A plot showing the data, together with the location of the mixture components, classification, uncertainty, and/or classification errors.

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References

C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611-631*.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

```
surfacePlot, clPairs, coordProj, mclust.options
```

Examples

mclustBIC

BIC for Model-Based Clustering

Description

BIC for parameterized Gaussian mixture models fitted by EM algorithm initialized by model-based hierarchical clustering.

Usage

Arguments

data

A numeric vector, matrix, or data frame of observations. Categorical variables are not allowed. If a matrix or data frame, rows correspond to observations and columns correspond to variables.

G

An integer vector specifying the numbers of mixture components (clusters) for which the BIC is to be calculated. The default is G=1:9, unless the argument x is specified, in which case the default is taken from the values associated with x.

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modelNames

A vector of character strings indicating the models to be fitted in the EM phase of clustering. The help file for mclustModelNames describes the available models. The default is:

c("E", "V") for univariate data

mclust.options("emModelNames") for multivariate data (n > d)

c("EII", "VII", "EEI", "EVI", "VEI", "VVI") the spherical and diagonal models for multivariate data (n <= d)

unless the argument x is specified, in which case the default is taken from the values associated with x.

prior

The default assumes no prior, but this argument allows specification of a conjugate prior on the means and variances through the function priorControl.

control

A list of control parameters for EM. The defaults are set by the call emControl().

initialization A list containing zero or more of the following components:

hcPairs A matrix of merge pairs for hierarchical clustering such as produced by function hc. For multivariate data, the default is to compute a hierarchical clustering tree by applying function hc with modelName = "VVV" to the data or a subset as indicated by the subset argument. The hierarchical clustering results are to start EM. For univariate data, the default is to use quantiles to start EM.

subset A logical or numeric vector specifying a subset of the data to be used in the initial hierarchical clustering phase.

noise A logical or numeric vector indicating an initial guess as to which observations are noise in the data. If numeric the entries should correspond to row indexes of the data. If supplied, a noise term will be added to the model in the estimation.

Vinv

An estimate of the reciprocal hypervolume of the data region. The default is determined by applying function hypvol to the data. Used only if an initial guess as to which observations are noise is supplied.

warn

A logical value indicating whether or not certain warnings (usually related to singularity) should be issued when estimation fails. The default is controlled by mclust.options.

Х

An object of class 'mclustBIC'. If supplied, mclustBIC will use the settings in x to produce another object of class 'mclustBIC', but with G and modelNames as specified in the arguments. Models that have already been computed in x are not recomputed. All arguments to mclustBIC except data, G and modelName are ignored and their values are set as specified in the attributes of x. Defaults for G and modelNames are taken from x.

... Catches unused arguments in indirect or list calls via do.call.

Value

Return an object of class 'mclustBIC' containing the Bayesian Information Criterion for the specified mixture models numbers of clusters. Auxiliary information returned as attributes.

The corresponding print method shows the matrix of values and the top models according to the BIC criterion.

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References

C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611:631*.

- C. Fraley and A. E. Raftery (2005). Bayesian regularization for normal mixture estimation and model-based clustering. Technical Report, Department of Statistics, University of Washington.
- C. Fraley and A. E. Raftery (2007). Bayesian regularization for normal mixture estimation and model-based clustering. *Journal of Classification* 24:155-181.
- C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

priorControl, emControl, mclustModel, summary.mclustBIC, hc, me, mclustModelNames, mclust.options

```
irisBIC <- mclustBIC(iris[,-5])</pre>
irisBIC
plot(irisBIC)
## Not run:
subset <- sample(1:nrow(iris), 100)</pre>
irisBIC <- mclustBIC(iris[,-5], initialization=list(subset = subset))</pre>
irisBIC
plot(irisBIC)
irisBIC1 <- mclustBIC(iris[,-5], G=seq(from=1,to=9,by=2),</pre>
                     modelNames=c("EII", "EEI", "EEE"))
irisBIC1
plot(irisBIC1)
irisBIC2 <- mclustBIC(iris[,-5], G=seq(from=2,to=8,by=2),</pre>
                        modelNames=c("VII", "VVI", "VVV"), x= irisBIC1)
irisBIC2
plot(irisBIC2)
## End(Not run)
nNoise <- 450
set.seed(0)
poissonNoise <- apply(apply( iris[,-5], 2, range), 2, function(x, n)</pre>
                       runif(n, min = x[1]-.1, max = x[2]+.1), n = nNoise)
set.seed(0)
noiseInit <- sample(c(TRUE,FALSE),size=nrow(iris)+nNoise,replace=TRUE,</pre>
                     prob=c(3,1)
irisNdata <- rbind(iris[,-5], poissonNoise)</pre>
irisNbic <- mclustBIC(data = irisNdata, G = 1:5,</pre>
                       initialization = list(noise = noiseInit))
irisNbic
plot(irisNbic)
```

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Mc	ustBootstran	i

Resampling-based Inference for Gaussian finite mixture models

Description

Bootstrap or jackknife estimation of standard errors and percentile bootstrap confidence intervals for the parameters of a Gaussian mixture model.

Usage

Arguments

object An object of class 'Mclust' or 'densityMclust' providing an estimated Gaus-

sian mixture model.

nboot The number of bootstrap replications.

type A character string specifying the type of resampling to use:

"bs" = nonparametric bootstrap "wlbs" = weighted likelihood bootstrap

"jk" = jackknife

verbose A logical, if TRUE and the session is interactive a text progress bar is displayed

during the bootstrap procedure.

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

Details

For a fitted Gaussian mixture model with object\$G mixture components and covariances parameterisation object\$modelName, this function returns either the boostrap distribution or the jackknife distribution of mixture parameters. In the former case, the nonparametric bootstrap or the weighted likelihood bootstrap approach could be used, so the the bootstrap procedure generates nboot bootstrap samples of the same size as the original data by resampling with replacement from the observed data. In the jackknife case, the procedure considers all the samples obtained by omitting one observation at time.

The resulting resampling distribution can then be used to obtain standard errors and percentile confidence intervals by the use of summary. MclustBootstrap function.

Value

An object of class 'MclustBootstrap' with the following components:

n The number of observations in the data.

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The dimension of the data. d G A value specifying the number of mixture components. modelName A character string specifying the mixture model covariances parameterisation (see mclustModelNames). A list of estimated parameters for the mixture components with the following parameters components: pro a vector of mixing proportions. mean a matrix of means for each component. variance an array of covariance matrices for each component. The number of bootstrap replications if type = "bs" or type = "wlbs". The nboot sample size if type = "jk". The type of resampling approach used. type nonfit The number of resamples that did not convergence during the procedure. A matrix of dimension (nboot x G) containing the bootstrap distribution for the pro mixing proportion. mean An array of dimension (nboot x d x G), where d is the dimension of the data, containing the bootstrap distribution for the component means.

References

variance

Davison A and Hinkley D (1907) Pactotuse Mathada and Their Applicat

Davison, A. and Hinkley, D. (1997) *Bootstrap Methods and Their Applications*. Cambridge University Press.

An array of dimension (nboot x d x d x d), where d is the dimension of the data,

containing the bootstrap distribution for the component covariances.

McLachlan, G.J. and Peel, D. (2000) Finite Mixture Models. Wiley.

O'Hagan A., Murphy T. B., Gormley I. C. and Scrucca L. (2015) On Estimation of Parameter Uncertainty in Model-Based Clustering. Submitted to *Computational Statistics*.

See Also

 $summary. \verb+MclustBootstrap+, \verb+plot+. \verb+MclustBootstrap+, \verb+Mclust+, density+ \verb+Mclust+.$

```
## Not run:
data(diabetes)
X = diabetes[,-1]
modClust = Mclust(X)
bootClust = MclustBootstrap(modClust)
summary(bootClust, what = "se")
summary(bootClust, what = "ci")

data(acidity)
modDens = densityMclust(acidity)
modDens = MclustBootstrap(modDens)
summary(modDens, what = "se")
```

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```
summary(modDens, what = "ci")
## End(Not run)
```

mclustBootstrapLRT

Bootstrap Likelihood Ratio Test for the Number of Mixture Components

Description

Perform the likelihood ratio test (LRT) for assessing the number of mixture components in a specific finite mixture model parameterisation. The observed significance is approximated by using the (parametric) bootstrap for the likelihood ratio test statistic (LRTS).

Usage

Arguments

data	A numeric vector, matrix, or data frame of observations. Categorical variables are not allowed. If a matrix or data frame, rows correspond to observations and columns correspond to variables.
modelName	A character string indicating the mixture model to be fitted. The help file for mclustModelNames describes the available models.
nboot	The number of bootstrap replications to use (by default 999).
level	The significance level to be used to terminate the sequential bootstrap procedure.
maxG	The maximum number of mixture components G to test. If not provided the procedure is stopped when a test is not significant at the specified level.
verbose	A logical, if TRUE and the session is interactive a text progress bar is displayed during the bootstrap procedure.
• • •	Further arguments passed to or from other methods. In particular, see the optional arguments in mclustBIC.
х	An 'mclustBootstrapLRT' object.
G	A value specifying the number of components for which to plot the bootstrap distribution.
hist.col	The colour to be used to fill the bars of the histogram.

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hist.border The color of the border around the bars of the histogram.

breaks See the argument in function hist.

col, lwd, lty The color, line width and line type to be used to represent the observed LRT

statistic.

main The title for the graph.

Details

The implemented algorithm for computing the LRT observed significance using the bootstrap is the following. Let G_0 be the number of mixture components under the null hypothesis versus $G_1 = G_0 + 1$ under the alternative. Bootstrap samples are drawn by simulating data under the null hypothesis. Then, the p-value may be approximated using eq. (13) on McLachlan and Rathnayake (2014). Equivalently, using the notation of Davison and Hinkley (1997) it may be computed as

$$\text{p-value} = \frac{1 + \#\{LRT_b^* \ge LRTS_{obs}\}}{B+1}$$

where

B = number of bootstrap samples

 LRT_{obs} = LRTS computed on the observed data

 LRT_b^* = LRTS computed on the *b*th bootstrap sample.

Value

An object of class 'mclustBootstrapLRT' with the following components:

G A vector of number of components tested under the null hypothesis.

modelName A character string specifying the mixture model as provided in the function call

(see above).

obs The observed values of the LRTS.

A matrix of dimension nboot x the number of components tested containing the

bootstrap values of LRTS.

p. value A vector of p-values.

References

Davison, A. and Hinkley, D. (1997) *Bootstrap Methods and Their Applications*. Cambridge University Press.

McLachlan G.J. (1987) On bootstrapping the likelihood ratio test statistic for the number of components in a normal mixture. *Applied Statistics*, 36, 318-324.

McLachlan, G.J. and Peel, D. (2000) Finite Mixture Models. Wiley.

McLachlan, G.J. and Rathnayake, S. (2014) On the number of components in a Gaussian mixture model. *Wiley Interdisciplinary Reviews: Data Mining and Knowledge Discovery*, 4(5), pp. 341-355.

See Also

mclustBIC, mclustICL, Mclust

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Examples

```
## Not run:
data(faithful)
faithful.boot = mclustBootstrapLRT(faithful, model = "VVV")
faithful.boot
plot(faithful.boot, G = 1)
plot(faithful.boot, G = 2)
## End(Not run)
```

MclustDA

MclustDA discriminant analysis

Description

Discriminant analysis based on Gaussian finite mixture modeling.

Usage

```
MclustDA(data, class, G = NULL, modelNames = NULL,
    modelType = c("MclustDA", "EDDA"),
    prior = NULL,
    control = emControl(),
    initialization = NULL,
    warn = mclust.options("warn"),
    ...)
```

Arguments

G

data A data frame or matrix giving the training data.

class A vector giving the class labels for the observations in the training data.

An integer vector specifying the numbers of mixture components (clusters) for which the BIC is to be calculated within each class. The default is G = 1:5.

A different set of mixture components for each class can be specified by providing this argument with a list of integers for each class. See the examples

below.

modelNames A vector of character strings indicating the models to be fitted by EM within

each class (see the description in mclustModelNames). A different set of mixture models for each class can be specified by providing this argument with a

list of character strings. See the examples below.

modelType A character string specifying whether the models given in modelNames should

fit a different number of mixture components and covariance structures for each class ("MclustDA", the default) or should be constrained to have a single component for each class with the same covariance structure among classes ("EDDA").

See Details section and the examples below.

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prior The default assumes no prior, but this argument allows specification of a conju-

gate prior on the means and variances through the function priorControl.

control A list of control parameters for EM. The defaults are set by the call emControl().

initialization A list containing zero or more of the following components:

hcPairs A matrix of merge pairs for hierarchical clustering such as produced by function hc. The default is to compute a hierarchical clustering tree by applying function hc with modelName = "E" to univariate data and modelName = "VVV" to multivariate data or a subset as indicated by the subset argument. The hierarchical clustering results are used as starting

subset A logical or numeric vector specifying a subset of the data to be used in the initial hierarchical clustering phase.

warn A logical value indicating whether or not certain warnings (usually related to

singularity) should be issued when estimation fails. The default is controlled by

mclust.options.

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

Details

The "EDDA" method for discriminant analysis is described in Bensmail and Celeux (1996), while "MclustDA" in Fraley and Raftery (2002).

Value

An object of class 'MclustDA' providing the optimal (according to BIC) mixture model.

The details of the output components are as follows:

call The matched call.
data The input data matrix.
class The input class labels.

type A character string specifying the modelType estimated.

models A list of Mclust objects containing information on fitted model for each class.

n The total number of observations in the data.

d The dimension of the data.

bic Optimal BIC value.

loglik Log-likelihood for the selected model.

df Number of estimated parameters.

References

Bensmail, H., and Celeux, G. (1996) Regularized Gaussian Discriminant Analysis Through Eigenvalue Decomposition. *Journal of the American Statistical Association*, 91, 1743-1748.

C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association*, 97, 611-631.

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C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

Author(s)

Luca Scrucca

See Also

summary.MclustDA, plot.MclustDA, predict.MclustDA, classError

```
odd \leftarrow seq(from = 1, to = nrow(iris), by = 2)
even \leftarrow odd + 1
X.train <- iris[odd,-5]</pre>
Class.train <- iris[odd,5]</pre>
X.test <- iris[even,-5]</pre>
Class.test <- iris[even,5]
# common EEE covariance structure (which is essentially equivalent to linear discriminant analysis)
irisMclustDA <- MclustDA(X.train, Class.train, modelType = "EDDA", modelNames = "EEE")</pre>
summary(irisMclustDA, parameters = TRUE)
summary(irisMclustDA, newdata = X.test, newclass = Class.test)
# common covariance structure selected by BIC
irisMclustDA <- MclustDA(X.train, Class.train, modelType = "EDDA")</pre>
summary(irisMclustDA, parameters = TRUE)
summary(irisMclustDA, newdata = X.test, newclass = Class.test)
# general covariance structure selected by BIC
irisMclustDA <- MclustDA(X.train, Class.train)</pre>
summary(irisMclustDA, parameters = TRUE)
summary(irisMclustDA, newdata = X.test, newclass = Class.test)
plot(irisMclustDA)
plot(irisMclustDA, dimens = 3:4)
plot(irisMclustDA, dimens = 4)
plot(irisMclustDA, what = "classification")
plot(irisMclustDA, what = "classification", newdata = X.test)
plot(irisMclustDA, what = "classification", dimens = 3:4)
plot(irisMclustDA, what = "classification", newdata = X.test, dimens = 3:4)
plot(irisMclustDA, what = "classification", dimens = 4)
plot(irisMclustDA, what = "classification", dimens = 4, newdata = X.test)
plot(irisMclustDA, what = "train&test", newdata = X.test)
plot(irisMclustDA, what = "train&test", newdata = X.test, dimens = 3:4)
plot(irisMclustDA, what = "train&test", newdata = X.test, dimens = 4)
plot(irisMclustDA, what = "error")
```

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```
plot(irisMclustDA, what = "error", dimens = 3:4)
plot(irisMclustDA, what = "error", dimens = 4)
plot(irisMclustDA, what = "error", newdata = X.test, newclass = Class.test)
plot(irisMclustDA, what = "error", newdata = X.test, newclass = Class.test, dimens = 3:4)
plot(irisMclustDA, what = "error", newdata = X.test, newclass = Class.test, dimens = 4)
## Not run:
# simulated 1D data
n <- 250
set.seed(1)
triModal <- c(rnorm(n,-5), rnorm(n,0), rnorm(n,5))
triClass \leftarrow c(rep(1,n), rep(2,n), rep(3,n))
odd <- seq(from = 1, to = length(triModal), by = 2)
even \leftarrow odd + 1
triMclustDA <- MclustDA(triModal[odd], triClass[odd])</pre>
summary(triMclustDA, parameters = TRUE)
summary(triMclustDA, newdata = triModal[even], newclass = triClass[even])
plot(triMclustDA, what = "scatterplot")
plot(triMclustDA, what = "classification")
plot(triMclustDA, what = "classification", newdata = triModal[even])
plot(triMclustDA, what = "train&test", newdata = triModal[even])
plot(triMclustDA, what = "error")
plot(triMclustDA, what = "error", newdata = triModal[even], newclass = triClass[even])
# simulated 2D cross data
data(cross)
odd \leftarrow seq(from = 1, to = nrow(cross), by = 2)
even \leftarrow odd + 1
crossMclustDA <- MclustDA(cross[odd,-1], cross[odd,1])</pre>
summary(crossMclustDA, parameters = TRUE)
summary(crossMclustDA, newdata = cross[even,-1], newclass = cross[even,1])
plot(crossMclustDA, what = "scatterplot")
plot(crossMclustDA, what = "classification")
plot(crossMclustDA, what = "classification", newdata = cross[even,-1])
plot(crossMclustDA, what = "train&test", newdata = cross[even,-1])
plot(crossMclustDA, what = "error")
plot(crossMclustDA, what = "error", newdata =cross[even,-1], newclass = cross[even,1])
## End(Not run)
```

MclustDR

Dimension reduction for model-based clustering and classification

Description

A dimension reduction method for visualizing the clustering or classification structure obtained from a finite mixture of Gaussian densities.

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Usage

Arguments

object An object of class 'Mclust' or 'MclustDA' resulting from a call to, respec-

tively, Mclust or MclustDA.

normalized Logical. If TRUE directions are normalized to unit norm.

Sigma Marginal covariance matrix of data. If not provided is estimated by the MLE of

observed data.

lambda A tuning parameter in the range [0,1] described in Scrucca (2014). The default

0.5 gives equal importance to differences in means and covariances among clusters/classes. To recover the directions that mostly separate the estimated clusters

or classes set this parameter to 1.

tol A tolerance value.

Details

The method aims at reducing the dimensionality by identifying a set of linear combinations, ordered by importance as quantified by the associated eigenvalues, of the original features which capture most of the clustering or classification structure contained in the data.

Information on the dimension reduction subspace is obtained from the variation on group means and, depending on the estimated mixture model, on the variation on group covariances (see Scrucca, 2010).

Observations may then be projected onto such a reduced subspace, thus providing summary plots which help to visualize the underlying structure.

The method has been extended to the supervised case, i.e. when the true classification is known (see Scrucca, 2013).

This implementation doesn't provide a formal procedure for the selection of dimensionality. A future release will include one or more methods.

Value

An object of class 'MclustDR' with the following components:

call The matched call

type A character string specifying the type of model for which the dimension reduc-

tion is computed. Currently, possible values are "Mclust" for clustering, and

"MclustDA" or "EDDA" for classification.

x The data matrix.

Sigma The covariance matrix of the data.

mixcomp A numeric vector specifying the mixture component of each data observation.

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class A factor specifying the classification of each data observation. For model-

based clustering this is equivalent to the corresponding mixture component. For

model-based classification this is the known classification.

G The number of mixture components.

modelName The name of the parameterization of the estimated mixture model(s). See mclustModelNames.

mu A matrix of means for each mixture component.

sigma An array of covariance matrices for each mixture component.

pro The estimated prior for each mixture component.

M The kernel matrix.

lambda The tuning parameter.

evalues The eigenvalues from the generalized eigen-decomposition of the kernel matrix.

raw.evectors The raw eigenvectors from the generalized eigen-decomposition of the kernel

matrix, ordered according to the eigenvalues.

basis The basis of the estimated dimension reduction subspace.

std.basis The basis of the estimated dimension reduction subspace standardized to vari-

ables having unit standard deviation.

numdir The dimension of the projection subspace.

dir The estimated directions, i.e. the data projected onto the estimated dimension

reduction subspace.

Author(s)

Luca Scrucca

References

Scrucca, L. (2010) Dimension reduction for model-based clustering. *Statistics and Computing*, 20(4), pp. 471-484.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

Scrucca, L. (2014) Graphical Tools for Model-based Mixture Discriminant Analysis. *Advances in Data Analysis and Classification*, 8(2), pp. 147-165

See Also

```
summary.MclustDR, plot.MclustDR, Mclust, MclustDA.
```

```
# clustering
data(diabetes)
mod = Mclust(diabetes[,-1])
summary(mod)
```

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```
dr = MclustDR(mod)
summary(dr)
plot(dr, what = "scatterplot")
plot(dr, what = "evalues")
# adjust the tuning parameter to show the most separating directions
dr1 = MclustDR(mod, lambda = 1)
summary(dr1)
plot(dr1, what = "scatterplot")
plot(dr1, what = "evalues")
# classification
data(banknote)
da = MclustDA(banknote[,2:7], banknote$Status, modelType = "EDDA")
dr = MclustDR(da)
summary(dr)
da = MclustDA(banknote[,2:7], banknote$Status)
dr = MclustDR(da)
summary(dr)
```

mclustICL

ICL Criterion for Model-Based Clustering

Description

ICL (Integrated Complete-data Likelihood) for parameterized Gaussian mixture models fitted by EM algorithm initialized by model-based hierarchical clustering.

Usage

Arguments

data

A numeric vector, matrix, or data frame of observations. Categorical variables are not allowed. If a matrix or data frame, rows correspond to observations and columns correspond to variables.

G

An integer vector specifying the numbers of mixture components (clusters) for which the criteria should be calculated. The default is G = 1:9.

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modelNames

A vector of character strings indicating the models to be fitted in the EM phase of clustering. The help file for mclustModelNames describes the available models. The default is:

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c("E", "V") for univariate data

mclust.options("emModelNames") for multivariate data (n > d)

c("EII", "VII", "EEI", "EVI", "VEI", "VVI") the spherical and diagonal models for multivariate data (n <= d)

initialization A list containing zero or more of the following components:

hcPairs A matrix of merge pairs for hierarchical clustering such as produced by function hc. For multivariate data, the default is to compute a hierarchical clustering tree by applying function hc with modelName = "VVV" to the data or a subset as indicated by the subset argument. The hierarchical clustering results are to start EM. For univariate data, the default is to use quantiles to start EM.

subset A logical or numeric vector specifying a subset of the data to be used in the initial hierarchical clustering phase.

Х

An object of class 'mclustICL'. If supplied, mclustICL will use the settings in x to produce another object of class 'mclustICL', but with G and modelNames as specified in the arguments. Models that have already been computed in x are not recomputed. All arguments to mclustICL except data, G and modelName are ignored and their values are set as specified in the attributes of x. Defaults for G and modelNames are taken from x.

. . .

Futher arguments used in the call to Mclust. See also mclustBIC.

object

An integer vector specifying the numbers of mixture components (clusters) for which the criteria should be calculated. The default is G = 1:9.

Value

Returns an object of class 'mclustICL' containing the the ICL criterion for the specified mixture models and numbers of clusters.

The corresponding print method shows the matrix of values and the top models according to the ICL criterion. The summary method shows only the top models.

References

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

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

plot.mclustICL, Mclust, mclustBIC, mclustBootstrapLRT, bic, icl

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Examples

```
data(faithful)
faithful.ICL <- mclustICL(faithful)
faithful.ICL
summary(faithful.ICL)
plot(faithful.ICL)
## Not run:
# compare with
faithful.BIC = mclustBIC(faithful)
faithful.BIC
plot(faithful.BIC)
## End(Not run)</pre>
```

mclustModel

Best model based on BIC

Description

Determines the best model from clustering via mclustBIC for a given set of model parameterizations and numbers of components.

Usage

```
mclustModel(data, BICvalues, G, modelNames, ...)
```

Arguments

data	The matrix or vector of observations used to generate 'object'.
BICvalues	An 'mclustBIC' object, which is the result of applying mclustBIC to data.
G	A vector of integers giving the numbers of mixture components (clusters) from which the best model according to BIC will be selected (as.character(G) must be a subset of the row names of BICvalues). The default is to select the best model for all numbers of mixture components used to obtain BICvalues.
modelNames	A vector of integers giving the model parameterizations from which the best model according to BIC will be selected (as.character(model) must be a subset of the column names of BICvalues). The default is to select the best model for parameterizations used to obtain BICvalues.
	Not used. For generic/method consistency.

Value

A list giving the optimal (according to BIC) parameters, conditional probabilities z, and log-likelihood, together with the associated classification and its uncertainty.

The details of the output components are as follows:

mclustModel 87

modelName	A character string indicating the model. The help file for ${\tt mclustModelNames}$ describes the available models.
n	The number of observations in the data.
d	The dimension of the data.
G	The number of components in the Gaussian mixture model corresponding to the optimal BIC.
bic	The optimal BIC value.
loglik	The log-likelihood corresponding to the optimal BIC.
parameters	A list with the following components:
	pro A vector whose <i>k</i> th component is the mixing proportion for the <i>k</i> th component of the mixture model. If missing, equal proportions are assumed.
	mean The mean for each component. If there is more than one component, this is a matrix whose kth column is the mean of the <i>k</i> th component of the mixture model.
	variance A list of variance parameters for the model. The components of this list depend on the model specification. See the help file for mclustVariance for details.
	Vinv The estimate of the reciprocal hypervolume of the data region used in the

A matrix whose [i,k]th entry is the probability that observation i in the test data belongs to the *k*th class.

the model.

computation when the input indicates the addition of a noise component to

References

Z

C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. Journal of the American Statistical Association 97:611-631.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

```
mclustBIC
```

```
irisBIC <- mclustBIC(iris[,-5])</pre>
mclustModel(iris[,-5], irisBIC)
mclustModel(iris[,-5], irisBIC, G = 1:6, modelNames = c("VII", "VVI", "VVV"))
```

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mclustModelNames

MCLUST Model Names

Description

Description of model names used in the MCLUST package.

Usage

```
mclustModelNames(model)
```

Arguments

model

A string specifying the model.

Details

The following models are available in package **mclust**:

univariate mixture		
"E"	=	equal variance (one-dimensional)
"V"	=	variable variance (one-dimensional)
multivariate mixture		
"EII"	=	spherical, equal volume
"VII"	=	spherical, unequal volume
"EEI"	=	diagonal, equal volume and shape
"VEI"	=	diagonal, varying volume, equal shape
"EVI"	=	diagonal, equal volume, varying shape
"VVI"	=	diagonal, varying volume and shape
"EEE"	=	ellipsoidal, equal volume, shape, and orientation
"EVE"	=	ellipsoidal, equal volume and orientation (*)
"VEE"	=	ellipsoidal, equal shape and orientation (*)
"VVE"	=	ellipsoidal, equal orientation (*)
"EEV"	=	ellipsoidal, equal volume and equal shape
"VEV"	=	ellipsoidal, equal shape
"EVV"	=	ellipsoidal, equal volume (*)
"VVV"	=	ellipsoidal, varying volume, shape, and orientation
single component		
"X"	=	univariate normal
"XII"	=	spherical multivariate normal
"XXI"	=	diagonal multivariate normal
"XXX"	=	ellipsoidal multivariate normal

^(*) new models in **mclust** version \geq 5.0.0.

mclustVariance 89

Value

Returns a list with the following components:

model a character string indicating the model (as in input).

type the description of the indicated model (see Details section).

References

C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611-631*.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

```
Mclust, mclustBIC
```

Examples

```
mclustModelNames("E")
mclustModelNames("EEE")
mclustModelNames("VVV")
mclustModelNames("XXXI")
```

mclustVariance

Template for variance specification for parameterized Gaussian mixture models

Description

Specification of variance parameters for the various types of Gaussian mixture models.

Usage

```
mclustVariance(modelName, d = NULL, G = 2)
```

Arguments

modelName A character string specifying the model.

d A integer specifying the dimension of the data.

G An integer specifying the number of components in the mixture model.

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Details

The variance component in the parameters list from the output to e.g. me or mstep or input to e.g. estep may contain one or more of the following arguments, depending on the model:

modelName A character string indicating the model.

- d The dimension of the data.
- G The number of components in the mixture model.
- sigmasq for the one-dimensional models ("E", "V") and spherical models ("EII", "VII"). This is either a vector whose *k*th component is the variance for the *k*th component in the mixture model ("V" and "VII"), or a scalar giving the common variance for all components in the mixture model ("E" and "EII").
- Sigma For the equal variance models "EII", "EEI", and "EEE". A d by d matrix giving the common covariance for all components of the mixture model.
- cholSigma For the equal variance model "EEE". A *d* by *d* upper triangular matrix giving the Cholesky factor of the common covariance for all components of the mixture model.
- sigma For all multidimensional mixture models. A d by d by G matrix array whose [,,k]th entry is the covariance matrix for the kth component of the mixture model.
- cholsigma For the unconstrained covariance mixture model "VVV". A *d* by *d* by *G* matrix array whose [,,k]th entry is the upper triangular Cholesky factor of the covariance matrix for the *k*th component of the mixture model.
- scale For diagonal models "EEI", "EVI", "VEI", "VVI" and constant-shape models "EEV" and "VEV". Either a *G*-vector giving the scale of the covariance (the *d*th root of its determinant) for each component in the mixture model, or a single numeric value if the scale is the same for each component.
- shape For diagonal models "EEI", "EVI", "VEI", "VVI" and constant-shape models "EEV" and "VEV". Either a G by d matrix in which the kth column is the shape of the covariance matrix (normalized to have determinant 1) for the kth component, or a d-vector giving a common shape for all components.
- orientation For the constant-shape models "EEV" and "VEV". Either a d by d by G array whose [,,k]th entry is the orthonomal matrix whose columns are the eigenvectors of the covariance matrix of the kth component, or a d by d orthonormal matrix if the mixture components have a common orientation. The orientation component is not needed in spherical and diagonal models, since the principal components are parallel to the coordinate axes so that the orientation matrix is the identity.

In all cases, the value -1 is used as a placeholder for unknown nonzero entries.

References

- C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611:631*.
- C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

me 91

models.	me	EM algorithm starting with M-step for parameterized MVN mixture models.
---------	----	---

Description

Implements the EM algorithm for MVN mixture models parameterized by eignevalue decomposition, starting with the maximization step.

Usage

```
me(modelName, data, z, prior = NULL, control = emControl(),
    Vinv = NULL, warn = NULL, ...)
```

Arguments

modelName	A character string indicating the model. The help file for mclustModelNames describes the available models.
data	A numeric vector, matrix, or data frame of observations. Categorical variables are not allowed. If a matrix or data frame, rows correspond to observations and columns correspond to variables.
Z	A matrix whose $[i,k]$ th entry is an initial estimate of the conditional probability of the ith observation belonging to the k th component of the mixture.
prior	Specification of a conjugate prior on the means and variances. See the help file for priorControl for further information. The default assumes no prior.
control	A list of control parameters for EM. The defaults are set by the call ${\tt emControl}$ ().
Vinv	If the model is to include a noise term, Vinv is an estimate of the reciprocal hypervolume of the data region. If set to a negative value or 0, the model will include a noise term with the reciprocal hypervolume estimated by the function hypvol. The default is not to assume a noise term in the model through the setting Vinv=NULL.
warn	A logical value indicating whether or not certain warnings (usually related to singularity) should be issued when the estimation fails. The default is set in mclust.options("warn").
	Catches unused arguments in indirect or list calls via do.call.

Value

A list including the following components:

modelName	A character string identifying the model (same as the input argument).
n	The number of observations in the data.
d	The dimension of the data.
G	The number of mixture components.

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z A matrix whose [i,k]th entry is the conditional probability of the *i*th observation belonging to the *k*th component of the mixture.

parameters

pro A vector whose *k*th component is the mixing proportion for the *k*th component of the mixture model. If the model includes a Poisson term for noise, there should be one more mixing proportion than the number of Gaussian components.

mean The mean for each component. If there is more than one component, this is a matrix whose kth column is the mean of the *k*th component of the mixture model.

variance A list of variance parameters for the model. The components of this list depend on the model specification. See the help file for mclustVariance for details.

Vinv The estimate of the reciprocal hypervolume of the data region used in the computation when the input indicates the addition of a noise component to the model.

loglik The log likelihood for the data in the mixture model.

control The list of control parameters for EM used.

prior The specification of a conjugate prior on the means and variances used, NULL if

no prior is used.

Attributes: "info" Information on the iteration.

"WARNING" An appropriate warning if problems are encountered in the compu-

tations.

References

C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association* 97:611-631.

C. Fraley and A. E. Raftery (2005). Bayesian regularization for normal mixture estimation and model-based clustering. Technical Report, Department of Statistics, University of Washington.

C. Fraley and A. E. Raftery (2007). Bayesian regularization for normal mixture estimation and model-based clustering. *Journal of Classification* 24:155-181.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

meE,..., meVVV, em, mstep, estep, priorControl, mclustModelNames, mclustVariance, mclust.options

```
me(modelName = "VVV", data = iris[,-5], z = unmap(iris[,5]))
```

me.weighted 93

me.weighted	EM algorithm with weights starting with M-step for parameterized MVN mixture models

Description

Implements the EM algorithm for fitting MVN mixture models parameterized by eigenvalue decomposition, when observations have weights, starting with the maximization step.

Usage

Arguments

modelName	A character string indicating the model. The help file for mclustModelNames describes the available models.
data	A numeric vector, matrix, or data frame of observations. Categorical variables are not allowed. If a matrix or data frame, rows correspond to observations and columns correspond to variables.
z	A matrix whose $[i,k]$ th entry is an initial estimate of the conditional probability of the ith observation belonging to the k th component of the mixture.
weights	A vector of positive weights, where the [i]th entry is the weight for the ith observation. If any of the weights are greater than one, then they are scaled so that the maximum weight is one.
prior	Specification of a conjugate prior on the means and variances. See the help file for priorControl for further information. The default assumes no prior.
control	A list of control parameters for EM. The defaults are set by the call emControl.
Vinv	If the model is to include a noise term, Vinv is an estimate of the reciprocal hypervolume of the data region. If set to a negative value or 0, the model will include a noise term with the reciprocal hypervolume estimated by the function hypvol. The default is not to assume a noise term in the model through the setting Vinv=NULL.
warn	A logical value indicating whether or not certain warnings (usually related to singularity) should be issued when the estimation fails. The default is set by warn using mclust.options.
	Catches unused arguments in indirect or list calls via do.call.

Value

A list including the following components:

modelName A character string identifying the model (same as the input argument).

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z A matrix whose [i,k]th entry is the conditional probability of the *i*th observation belonging to the *k*th component of the mixture.

parameters

pro A vector whose *k*th component is the mixing proportion for the *k*th component of the mixture model. If the model includes a Poisson term for noise, there should be one more mixing proportion than the number of Gaussian components.

mean The mean for each component. If there is more than one component, this is a matrix whose kth column is the mean of the *k*th component of the mixture model.

variance A list of variance parameters for the model. The components of this list depend on the model specification. See the help file for mclustVariance for details.

Vinv The estimate of the reciprocal hypervolume of the data region used in the computation when the input indicates the addition of a noise component to the model.

loglik The log likelihood for the data in the mixture model.

Attributes: "info" Information on the iteration.

"WARNING" An appropriate warning if problems are encountered in the computations.

References

- C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association* 97:611-631.
- C. Fraley and A. E. Raftery (2005). Bayesian regularization for normal mixture estimation and model-based clustering. Technical Report, Department of Statistics, University of Washington.
- C. Fraley and A. E. Raftery (2007). Bayesian regularization for normal mixture estimation and model-based clustering. *Journal of Classification* 24:155-181.
- C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

Author(s)

Thomas Brendan Murphy

See Also

me, meE,..., meVVV, em, mstep, estep, priorControl, mclustModelNames, mclustVariance, mclust.options

```
w \leftarrow rep(1,150)

w[1] \leftarrow 0

me.weighted(modelName = "VVV", data = iris[,-5], z = unmap(iris[,5]),weights=w)
```

meE 95

meE

EM algorithm starting with M-step for a parameterized Gaussian mixture model.

Description

Implements the EM algorithm for a parameterized Gaussian mixture model, starting with the maximization step.

Usage

```
meE(data, z, prior=NULL, control=emControl(), Vinv=NULL, warn=NULL, ...)
meV(data, z, prior=NULL, control=emControl(), Vinv=NULL, warn=NULL, ...)
meX(data, prior = NULL, warn = NULL, ...)
meEII(data, z, prior=NULL, control=emControl(), Vinv=NULL, warn=NULL, ...)
meVII(data, z, prior=NULL, control=emControl(), Vinv=NULL, warn=NULL, ...)
meEEI(data, z, prior=NULL, control=emControl(), Vinv=NULL, warn=NULL, ...)
meVEI(data, z, prior=NULL, control=emControl(), Vinv=NULL, warn=NULL, ...)
meEVI(data, z, prior=NULL, control=emControl(), Vinv=NULL, warn=NULL, ...)
meVVI(data, z, prior=NULL, control=emControl(), Vinv=NULL, warn=NULL, ...)
meEEE(data, z, prior=NULL, control=emControl(), Vinv=NULL, warn=NULL, ...)
meEVE(data, z, prior=NULL, control=emControl(), Vinv=NULL, warn=NULL, ...)
meVEE(data, z, prior=NULL, control=emControl(), Vinv=NULL, warn=NULL, ...)
meVVE(data, z, prior=NULL, control=emControl(), Vinv=NULL, warn=NULL, ...)
meEEV(data, z, prior=NULL, control=emControl(), Vinv=NULL, warn=NULL, ...)
meVEV(data, z, prior=NULL, control=emControl(), Vinv=NULL, warn=NULL, ...)
meEVV(data, z, prior=NULL, control=emControl(), Vinv=NULL, warn=NULL, ...)
meVVV(data, z, prior=NULL, control=emControl(), Vinv=NULL, warn=NULL, ...)
meXII(data, prior = NULL, warn = NULL, ...)
meXXI(data, prior = NULL, warn = NULL, ...)
meXXX(data, prior = NULL, warn = NULL, ...)
```

Arguments

data	A numeric vector, matrix, or data frame of observations. Categorical variables are not allowed. If a matrix or data frame, rows correspond to observations and columns correspond to variables.
Z	A matrix whose $[i,k]$ th entry is the conditional probability of the ith observation belonging to the k th component of the mixture.
prior	Specification of a conjugate prior on the means and variances. The default assumes no prior.
control	A list of control parameters for EM. The defaults are set by the call emControl().
Vinv	An estimate of the reciprocal hypervolume of the data region, when the model is to include a noise term. Set to a negative value or zero if a noise term is desired, but an estimate is unavailable — in that case function hypvol will be used to obtain the estimate. The default is not to assume a noise term in the model through the setting Vinv=NULL.

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warn A logical value indicating whether or not certain warnings (usually related to

singularity) should be issued when the estimation fails. The default is given by

mclust.options("warn").

... Catches unused arguments in indirect or list calls via do. call.

Value

A list including the following components:

modelName A character string identifying the model (same as the input argument).

z A matrix whose [i,k]th entry is the conditional probability of the *i*th observa-

tion belonging to the kth component of the mixture.

parameters pro A vector whose kth component is the mixing proportion for the kth component of the mixture model. If the model includes a Poisson term for noise,

there should be one more mixing proportion than the number of Gaussian

components.

mean The mean for each component. If there is more than one component, this is a matrix whose kth column is the mean of the kth component of the

mixture model

variance A list of variance parameters for the model. The components of this list depend on the model specification. See the help file for mclustVariance

for details.

Vinv The estimate of the reciprocal hypervolume of the data region used in the

computation when the input indicates the addition of a noise component to

the model.

loglik The log likelihood for the data in the mixture model.

Attributes: "info" Information on the iteration.

"WARNING" An appropriate warning if problems are encountered in the compu-

tations.

References

C. Fraley and A. E. Raftery (2002a). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611-631*.

C. Fraley and A. E. Raftery (2005). Bayesian regularization for normal mixture estimation and model-based clustering. Technical Report, Department of Statistics, University of Washington.

C. Fraley and A. E. Raftery (2007). Bayesian regularization for normal mixture estimation and model-based clustering. *Journal of Classification* 24:155-181.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

em, me, estep, mclust.options

mstep 97

Examples

```
meVVV(data = iris[,-5], z = unmap(iris[,5]))
```

mstep

M-step for parameterized Gaussian mixture models.

Description

Maximization step in the EM algorithm for parameterized Gaussian mixture models.

Usage

```
mstep(modelName, data, z, prior = NULL, warn = NULL, ...)
```

Arguments

modelName	A character string indicating the model. The help file for mclustModelNames describes the available models.
data	A numeric vector, matrix, or data frame of observations. Categorical variables are not allowed. If a matrix or data frame, rows correspond to observations and columns correspond to variables.
Z	A matrix whose [i,k]th entry is the conditional probability of the ith observation belonging to the <i>k</i> th component of the mixture. In analyses involving noise, this should not include the conditional probabilities for the noise component.
prior	Specification of a conjugate prior on the means and variances. The default assumes no prior.
warn	A logical value indicating whether or not certain warnings (usually related to singularity) should be issued when the estimation fails. The default is given by mclust.options("warn").
	Catches unused arguments in indirect or list calls via do.call.

Value

A list including the following components:

modelName A character string iden

.

A character string identifying the model (same as the input argument).

parameters

pro A vector whose *k*th component is the mixing proportion for the *k*th component of the mixture model. If the model includes a Poisson term for noise, there should be one more mixing proportion than the number of Gaussian components.

mean The mean for each component. If there is more than one component, this is a matrix whose kth column is the mean of the *k*th component of the mixture model.

variance A list of variance parameters for the model. The components of this list depend on the model specification. See the help file for mclustVariance for details.

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Attributes:

"info" For those models with iterative M-steps ("VEI" and "VEV"), information on the iteration.

"WARNING" An appropriate warning if problems are encountered in the computations.

References

C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611-631*.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

Note

This function computes the M-step only for MVN mixtures, so in analyses involving noise, the conditional probabilities input should exclude those for the noise component.

In contrast to me for the EM algorithm, computations in mstep are carried out unless failure due to overflow would occur. To impose stricter tolerances on a single mstep, use me with the *itmax* component of the control argument set to 1.

See Also

```
mstepE, ..., mstepVVV, emControl, me, estep, mclust.options.
```

Examples

```
mstep(modelName = "VII", data = iris[,-5], z = unmap(iris[,5]))
```

mstepE

M-step for a parameterized Gaussian mixture model.

Description

Maximization step in the EM algorithm for a parameterized Gaussian mixture model.

Usage

```
mstepE( data, z, prior = NULL, warn = NULL, ...)
mstepV( data, z, prior = NULL, warn = NULL, ...)
mstepEII( data, z, prior = NULL, warn = NULL, ...)
mstepVII( data, z, prior = NULL, warn = NULL, ...)
mstepEEI( data, z, prior = NULL, warn = NULL, ...)
mstepVEI( data, z, prior = NULL, warn = NULL, control = NULL, ...)
mstepEVI( data, z, prior = NULL, warn = NULL, ...)
mstepVVI( data, z, prior = NULL, warn = NULL, ...)
```

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```
mstepEEE( data, z, prior = NULL, warn = NULL, ...)
mstepEEV( data, z, prior = NULL, warn = NULL, ...)
mstepVEV( data, z, prior = NULL, warn = NULL, control = NULL,...)
mstepVVV( data, z, prior = NULL, warn = NULL, ...)
mstepEVE( data, z, prior = NULL, warn = NULL, control = NULL, ...)
mstepEVV( data, z, prior = NULL, warn = NULL, ...)
mstepVEE( data, z, prior = NULL, warn = NULL, control = NULL, ...)
mstepVVE( data, z, prior = NULL, warn = NULL, control = NULL, ...)
```

Arguments

data A numeric vector, matrix, or data frame of observations. Categorical variables are not allowed. If a matrix or data frame, rows correspond to observations and

columns correspond to variables.

A matrix whose [i,k]th entry is the conditional probability of the ith observa-Z tion belonging to the kth component of the mixture. In analyses involving noise,

this should not include the conditional probabilities for the noise component.

prior Specification of a conjugate prior on the means and variances. The default as-

sumes no prior.

A logical value indicating whether or not certain warnings (usually related to warn

singularity) should be issued when the estimation fails. The default is given by

mclust.options("warn").

control Values controlling termination for models "VEI" and "VEV" that have an it-

erative M-step. This should be a list with components named itmax and tol. These components can be of length 1 or 2; in the latter case, mstep will use the second value, under the assumption that the first applies to an outer iteration (as in the function me). The default uses the default values from the function emControl, which sets no limit on the number of iterations, and a relative toler-

ance of sqrt(.Machine\$double.eps) on successive iterates.

Catches unused arguments in indirect or list calls via do. call.

Value

A list including the following components:

A character string identifying the model (same as the input argument). modelName

parameters pro A vector whose kth component is the mixing proportion for the kth compo-

nent of the mixture model. If the model includes a Poisson term for noise, there should be one more mixing proportion than the number of Gaussian

components.

mean The mean for each component. If there is more than one component, this is a matrix whose kth column is the mean of the kth component of the

mixture model.

variance A list of variance parameters for the model. The components of this list depend on the model specification. See the help file for mclustVariance for details.

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Attributes:

"info" For those models with iterative M-steps ("VEI" and "VEV"), information

on the iteration.

"WARNING" An appropriate warning if problems are encountered in the compu-

tations.

References

C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611-631*.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

Note

This function computes the M-step only for MVN mixtures, so in analyses involving noise, the conditional probabilities input should exclude those for the noise component.

In contrast to me for the EM algorithm, computations in mstep are carried out unless failure due to overflow would occur. To impose stricter tolerances on a single mstep, use me with the *itmax* component of the control argument set to 1.

See Also

```
mstep, me, estep, mclustVariance, priorControl, emControl.
```

Examples

```
mstepVII(data = iris[,-5], z = unmap(iris[,5]))
```

mvn

Univariate or Multivariate Normal Fit

Description

Computes the mean, covariance, and log-likelihood from fitting a single Gaussian to given data (univariate or multivariate normal).

Usage

```
mvn( modelName, data, prior = NULL, warn = NULL, ...)
```

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Arguments

modelName A character string representing a model name. This can be either "Spherical",

"Diagonal", or "Ellipsoidal" or else

"X" for one-dimensional data,
"XII" for a spherical Gaussian,
"XXI" for a diagonal Gaussian

"XXX" for a general ellipsoidal Gaussian

data A numeric vector, matrix, or data frame of observations. Categorical variables

are not allowed. If a matrix or data frame, rows correspond to observations and

columns correspond to variables.

prior Specification of a conjugate prior on the means and variances. The default as-

sumes no prior.

warn A logical value indicating whether or not a warning should be issued whenever a

singularity is encountered. The default is given by mclust.options("warn").

... Catches unused arguments in indirect or list calls via do.call.

Value

A list including the following components:

modelName A character string identifying the model (same as the input argument).

parameters mean The mean for each component. If there is more than one component,

this is a matrix whose kth column is the mean of the kth component of the

mixture model.

variance A list of variance parameters for the model. The components of this

list depend on the model specification. See the help file for mclustVariance

for details.

loglik The log likelihood for the data in the mixture model.

Attributes: "WARNING" An appropriate warning if problems are encountered in the compu-

tations.

References

C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association* 97:611-631.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

mvnX, mvnXII, mvnXXI, mvnXXX, mclustModelNames

mvnX

Examples

```
n <- 1000
set.seed(0)
x \leftarrow rnorm(n, mean = -1, sd = 2)
mvn(modelName = "X", x)
mu < -c(-1, 0, 1)
set.seed(0)
x <- sweep(matrix(rnorm(n*3), n, 3) %*% (2*diag(3)),</pre>
           MARGIN = 2, STATS = mu, FUN = "+")
mvn(modelName = "XII", x)
mvn(modelName = "Spherical", x)
set.seed(0)
x \leftarrow sweep(matrix(rnorm(n*3), n, 3) %*% diag(1:3),
           MARGIN = 2, STATS = mu, FUN = "+")
mvn(modelName = "XXI", x)
mvn(modelName = "Diagonal", x)
Sigma \leftarrow matrix(c(9,-4,1,-4,9,4,1,4,9), 3, 3)
set.seed(0)
x <- sweep(matrix(rnorm(n*3), n, 3) %*% chol(Sigma),</pre>
           MARGIN = 2, STATS = mu, FUN = "+")
mvn(modelName = "XXX", x)
mvn(modelName = "Ellipsoidal", x)
```

mvnX

Univariate or Multivariate Normal Fit

Description

Computes the mean, covariance, and log-likelihood from fitting a single Gaussian (univariate or multivariate normal).

Usage

```
mvnX(data, prior = NULL, warn = NULL, ...)
mvnXII(data, prior = NULL, warn = NULL, ...)
mvnXXI(data, prior = NULL, warn = NULL, ...)
mvnXXX(data, prior = NULL, warn = NULL, ...)
```

Arguments

data

A numeric vector, matrix, or data frame of observations. Categorical variables are not allowed. If a matrix or data frame, rows correspond to observations and columns correspond to variables.

mvnX 103

prior	Specification of a conjugate prior on the means and variances. The default assumes no prior.
warn	A logical value indicating whether or not a warning should be issued whenever a singularity is encountered. The default is given by mclust.options("warn").
	Catches unused arguments in indirect or list calls via do.call.

Details

mvnXII computes the best fitting Gaussian with the covariance restricted to be a multiple of the identity.

mvnXXI computes the best fitting Gaussian with the covariance restricted to be diagonal. mvnXXX computes the best fitting Gaussian with ellipsoidal (unrestricted) covariance.

Value

A list including the following components:

modelName A character string identifying the model (same as the input argument).

parameters mean The mean for each component. If there is more than one component,

this is a matrix whose kth column is the mean of the kth component of the

mixture model.

variance A list of variance parameters for the model. The components of this list depend on the model specification. See the help file for mclustVariance

for details.

loglik The log likelihood for the data in the mixture model.

Attributes: "WARNING" An appropriate warning if problems are encountered in the compu-

tations.

References

C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611-631*.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

```
mvn, mstepE
```

```
n <- 1000
set.seed(0)
x <- rnorm(n, mean = -1, sd = 2)
mvnX(x)</pre>
```

104 nMclustParams

nMclustParams

Number of Estimated Parameters in Gaussian Mixture Models

Description

Gives the number of estimated parameters for parameterizations of the Gaussian mixture model that are used in MCLUST.

Usage

```
nMclustParams(modelName, d, G, noise = FALSE, equalPro = FALSE, ...)
```

Arguments

modelName	A character string indicating the model. The help file for mclustModelNames describes the available models.
d	The dimension of the data. Not used for models in which neither the shape nor the orientation varies.
G	The number of components in the Gaussian mixture model used to compute loglik.
noise	A logical variable indicating whether or not the model includes an optional Poisson noise component.
equalPro	A logical variable indicating whether or not the components in the model are assumed to be present in equal proportion.
	Catches unused arguments in indirect or list calls via do.call.

Details

To get the total number of parameters in model, add G*d for the means and G-1 for the mixing proportions if they are unequal.

nVarParams 105

Value

The number of variance parameters in the corresponding Gaussian mixture model.

References

C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611:631*.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

bic, nVarParams.

Examples

```
mapply(nMclustParams, mclust.options("emModelNames"), d = 2, G = 3)
```

nVarParams

Number of Variance Parameters in Gaussian Mixture Models

Description

Gives the number of variance parameters for parameterizations of the Gaussian mixture model that are used in MCLUST.

Usage

```
nVarParams(modelName, d, G, ...)
```

Arguments

modelName	A character string indicating the model. The help file for mclustModelNames describes the available models.
d	The dimension of the data. Not used for models in which neither the shape nor the orientation varies.
G	The number of components in the Gaussian mixture model used to compute loglik.
	Catches unused arguments in indirect or list calls via do.call.

Details

To get the total number of parameters in model, add G*d for the means and G-1 for the mixing proportions if they are unequal.

106 partconv

Value

The number of variance parameters in the corresponding Gaussian mixture model.

References

C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611:631*.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

bic, nMclustParams.

Examples

```
mapply(nVarParams, mclust.options("emModelNames"), d = 2, G = 3)
```

partconv

Numeric Encoding of a Partitioning

Description

Converts a vector interpreted as a classification or partitioning into a numeric vector.

Usage

```
partconv(x, consec=TRUE)
```

Arguments

x A vector interpreted as a classification or partitioning.

consec Logical value indicating whether or not to consecutive class numbers should be

used.

Value

Numeric encoding of x. When consec = TRUE, the distinct values in x are numbered by the order in which they appear. When consec = FALSE, each distinct value in x is numbered by the index corresponding to its first appearance in x.

See Also

partuniq

partuniq 107

Examples

```
partconv(iris[,5])
set.seed(0)
cl <- sample(LETTERS[1:9], 25, replace=TRUE)
partconv(cl, consec=FALSE)
partconv(cl, consec=TRUE)</pre>
```

partuniq

Classifies Data According to Unique Observations

Description

Gives a one-to-one mapping from unique observations to rows of a data matrix.

Usage

```
partuniq(x)
```

Arguments

х

Matrix of observations.

Value

A vector of length nrow(x) with integer entries. An observation k is assigned an integer i whenever observation i is the first row of x that is identical to observation k (note that i \leq k).

See Also

```
partconv
```

```
set.seed(0)
mat <- data.frame(lets = sample(LETTERS[1:2],9,TRUE), nums = sample(1:2,9,TRUE))
mat
ans <- partuniq(mat)
ans
partconv(ans,consec=TRUE)</pre>
```

108 plot.clustCombi

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Plot Combined Clusterings Results

Description

Plot combined clusterings results: classifications corresponding to Mclust/BIC and to the hierarchically combined classes, and "entropy plots" to help to select a number of classes.

Usage

```
## S3 method for class 'clustCombi'
plot(x, data = NULL, what = c("classification", "entropy"), reg = 2, ...)
```

Arguments

X	Output from clustCombi.
^	Output from clustcomor.
data	The data used to produce Output.
what	Choose one or more of: "classification", "entropy".
reg	The number of parts of the piecewise linear regression for the entropy plots. Choose one or more of : 2 (for 1 change-point), 3 (for 2 change-points).
•••	Other arguments to be passed to combiPlot, entPlot, or to the Mclust called plot functions (please see the corresponding documentations).

Value

Classifications are plotted with combiPlot, which relies on the Mclust plot functions. Entropy plots (plotted with entPlot) may help to select a number of classes: please see the article cited in the references.

Author(s)

```
J.-P. Baudry, A. E. Raftery, L. Scrucca
```

References

J.-P. Baudry, A. E. Raftery, G. Celeux, K. Lo and R. Gottardo (2010). Combining mixture components for clustering. *Journal of Computational and Graphical Statistics*, 19(2):332-353.

See Also

```
combiPlot, entPlot, clustCombi
```

plot.densityMclust 109

Examples

```
## Not run:
data(Baudry_etal_2010_JCGS_examples)
## 1D Example
output <- clustCombi(Test1D, G=1:15)</pre>
# plots the hierarchy of combined solutions, then some "entropy plots" which
# may help one to select the number of classes (please see the article cited
# in the references)
plot(output, Test1D)
## 2D Example
output <- clustCombi(ex4.1)</pre>
# plots the hierarchy of combined solutions, then some "entropy plots" which
# may help one to select the number of classes (please see the article cited
# in the references)
plot(output, ex4.1)
## 3D Example
output <- clustCombi(ex4.4.2)</pre>
# plots the hierarchy of combined solutions, then some "entropy plots" which
# may help one to select the number of classes (please see the article cited
# in the references)
plot(output, ex4.4.2)
## End(Not run)
```

plot.densityMclust

Plots for Mixture-Based Density Estimate

Description

Plotting methods for an object of class 'mclustDensity'. Available graphs are plot of BIC values and density for univariate and bivariate data. For higher data dimensionality a scatterplot matrix of pairwise densities is drawn.

Usage

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```
points.pch = 1, points.col = 1, points.cex = 0.8, ...)
plotDensityMclustd(x, data = NULL, nlevels = 11, levels = NULL, col = grey(0.6),
                   points.pch = 1, points.col = 1, points.cex = 0.8,
                   gap = 0.2, ...)
```

Arguments

An object of class 'mclustDensity' obtained from a call to densityMclust Х

function.

Optional data points. data

The type of graph requested: what

"density" = a plot of estimated density; if data is also provided the density is

plotted over data points (see Details section).

"BIC" = a plot of BIC values for the estimated models versus the number of

components.

"diagnostic" = diagnostic plots (only available for the one-dimensional case,

see densityMclust.diagnostic)

hist.col The color to be used to fill the bars of the histogram.

hist.border The color of the border around the bars of the histogram.

breaks See the argument in function hist.

points.pch, points.col, points.cex

The character symbols, colors, and magnification to be used for plotting data

points.

An integer, the number of levels to be used in plotting contour densities. nlevels

levels A vector of density levels at which to draw the contour lines.

col Color to be used for drawing the contour lines, the perspective plot, or the image

density. In the latter case can be also a vector of color values.

Distance between subplots, in margin lines, for the matrix of pairwise scattergap

plots.

Additional arguments. . . .

Details

The function plot densityMclust allows to obtain the plot of estimated density or the graph of BIC values for evaluated models.

If what = "density" the produced plot dependes on the dimensionality of the data.

For one-dimensional data a call with no data provided produces a plot of the estimated density over a sensible range of values. If data is provided the density is over-plotted on a histogram for the observed data.

For two-dimensional data further arguments available are those accepted by the surfacePlot function. In particular, the density can be represented through "contour", "image", and "persp" type of graph.

For higher dimensionality a scatterplot matrix of pairwise densities is drawn.

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References

C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611:631*.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

Author(s)

Luca Scrucca

See Also

densityMclust, densityMclust.diagnostic, Mclust.

Examples

```
dens = densityMclust(faithful$waiting)
plot(dens, what = "density")
plot(dens, what = "density", data = faithful$waiting)
dens = densityMclust(faithful)
plot(dens, what = "density")
plot(dens, what = "density", type = "image", col = "steelblue")
plot(dens, what = "density", type = "persp", col = adjustcolor("steelblue", alpha.f = 0.5))
x = iris[,1:4]
dens = densityMclust(x)
plot(dens, what = "density", nlevels = 7)
## Not run:
  plot(dens, x, what = "density", drawlabels = FALSE,
       levels = quantile(dens$density, probs = c(0.05, 0.25, 0.5, 0.75, 0.95)))
  plot(dens, what = "density", type = "image", col = "steelblue")
 plot(dens, what = "density", type = "persp", border = adjustcolor(grey(0.1), alpha.f = 0.5))
## End(Not run)
```

plot.Mclust

Plot Model-Based Clustering Results

Description

Plot model-based clustering results: BIC, classification, uncertainty and (for univariate and bivariate data) density.

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Usage

```
## S3 method for class 'Mclust'
plot(x, what = c("BIC", "classification", "uncertainty", "density"),
    dimens = NULL, xlab = NULL, ylab = NULL, ylim = NULL,
    addEllipses = TRUE, main = TRUE, ...)
```

Arguments

x Output from Mclust.

what The type of graph requested:

"BTC"

"classification"
"uncertainty"
"density"

By default, all the above graphs are produced. See the description below.

dimens A vector of length one or two giving the integer dimensions of the desired

coordinate projections for multivariate data in case of "classification" or

"uncertainty" plots.

xlab, ylab Optional labels for the x-axis and the y-axis.

ylim Optional limits for the vertical axis of the BIC plot.

addEllipses A logical indicating whether or not to add ellipses with axes corresponding to

the within-cluster covariances in case of "classification" or "uncertainty"

plots.

main A logical or NULL indicating whether or not to add a title to the plot identifying

the dimensions used.

... Other graphics parameters.

Details

For more flexibility in plotting, use mclust1Dplot, mclust2Dplot, surfacePlot, coordProj, or randProj.

Value

Model-based clustering plots:

"BIC" = BIC values used for choosing the number of clusters.

"classification" = a plot showing the clustering. For data in more than two dimensions a pairs plot is produced, followed by a coordinate projection plot using specified dimens.

"uncertainty" = a plot of classification uncertainty. For data in more than two dimensions a coordinate projection plot is drawn using specified dimens.

"density" = a plot of estimated density. For two dimensional a contour plot is drawn, while for data in more than two dimensions a matrix of contours for pairs of variables is produced.

plot.mclustBIC 113

References

C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association* 97:611-631.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

Mclust, plot.mclustBIC, plot.mclustICL, mclust1Dplot, mclust2Dplot, surfacePlot, coordProj, randProj.

Examples

```
precipMclust <- Mclust(precip)
plot(precipMclust)

faithfulMclust <- Mclust(faithful)
plot(faithfulMclust)

irisMclust <- Mclust(iris[,-5])
plot(irisMclust)</pre>
```

plot.mclustBIC

BIC Plot for Model-Based Clustering

Description

Plots the BIC values returned by the mclustBIC function.

Usage

```
## S3 method for class 'mclustBIC'
plot(x, G = NULL, modelNames = NULL,
    symbols = NULL, colors = NULL,
    xlab = NULL, ylab = "BIC", ylim = NULL,
    legendArgs = list(x = "bottomright", ncol = 2, cex = 1, inset = 0.01),
    ...)
```

Arguments

X	Output from mclustBIC
Х	Output from metustbic

G One or more numbers of components corresponding to models fit in x. The

default is to plot the BIC for all of the numbers of components fit.

modelNames One or more model names corresponding to models fit in x. The default is to

plot the BIC for all of the models fit.

plot.mclustBIC

symbols	Either an integer or character vector assigning a plotting symbol to each unique class in classification. Elements in colors correspond to classes in order of appearance in the sequence of observations (the order used by the function unique). The default is given by mclust.options("classPlotSymbols").
colors	Either an integer or character vector assigning a color to each unique class in classification. Elements in colors correspond to classes in order of appearance in the sequence of observations (the order used by the function unique). The default is given by mclust.options("classPlotColors").
xlab	Optional label for the horizontal axis of the BIC plot.
ylab	Label for the vertical axis of the BIC plot.
ylim	Optional limits for the vertical axis of the BIC plot.
legendArgs	Arguments to pass to the legend function. Set to NULL for no legend.
	Other graphics parameters.

Value

A plot of the BIC values.

References

- C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611-631*.
- C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

mclustBIC

```
## Not run:
plot(mclustBIC(precip), legendArgs = list(x = "bottomleft"))
plot(mclustBIC(faithful))
plot(mclustBIC(iris[,-5]))
## End(Not run)
```

plot.MclustBootstrap 115

Description

Plots the bootstrap distribution of parameters as returned by the MclustBootstrap function.

Usage

```
## S3 method for class 'MclustBootstrap'
plot(x, what = c("pro", "mean", "var"),
    hist.col = "grey", hist.border = "lightgrey", breaks = "Sturges",
    col = "forestgreen", lwd = 2, lty = 3,
    xlab = NULL, xlim = NULL, ylim = NULL, ...)
```

Arguments

X	Object returned by MclustBootstrap.
what	Character string specifying if mixing proportions ("pro"), component means ("mean") or component variances ("var") should be drawn.
hist.col	The color to be used to fill the bars of the histograms.
hist.border	The color of the border around the bars of the histograms.
breaks	See the argument in function hist.
col, lwd, lty	The color, line width and line type to be used to represent the estimated parameters.
xlab	Optional label for the horizontal axis.
xlim, ylim	A two-values vector of axis range for, respectively, horizontal and vertical axis.
	Other graphics parameters.

Value

A plot for each variable/component of the selected parameters.

See Also

```
MclustBootstrap
```

```
data(diabetes)
X = diabetes[,-1]
modClust = Mclust(X, G = 3, modelNames = "VVV")
bootClust = MclustBootstrap(modClust, nboot = 99)
par(mfrow = c(1,3), mar = c(4,2,2,0.5))
plot(bootClust, what = "pro")
par(mfrow = c(3,3), mar = c(4,2,2,0.5))
plot(bootClust, what = "mean")
```

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Plotting method for MclustDA discriminant analysis

Description

Graphical tools for training and test data, known training data classification, mclustDA test data classification, and/or training errors.

Usage

```
## S3 method for class 'MclustDA'
plot(x, what = c("scatterplot", "classification", "train&test", "error"),
    newdata, newclass, dimens, symbols, colors, ...)
```

Arguments

x An object of class 'MclustDA' resulting from a call to MclustDA.

what The type of graph requested:

"scatterplot" = a plot of training data with points marked based the known classification. Ellipses corresponding to covariances of mixture components are also drawn.

"classification" = a plot of data with points marked based the predicted classification; if newdata is provided then the test set is shown otherwise the training set.

"train&test" = a plot of training and test data with points marked according to the type of set.

"error" = a plot of training set (or test set if newdata and newclass are provided) with misclassified points marked.

newdata A data frame or matrix for test data.

newclass A vector giving the class labels for the observations in the test data (if known).

dimens A vector of integers giving the dimensions of the desired coordinate projections for multivariate data. The default is to take all the the available dimensions for

plotting.

symbols Either an integer or character vector assigning a plotting symbol to each unique

class. Elements in colors correspond to classes in order of appearance in the sequence of observations (the order used by the function factor). The default

is given by mclust.options("classPlotSymbols").

colors Either an integer or character vector assigning a color to each unique class in

classification. Elements in colors correspond to classes in order of appearance in the sequence of observations (the order used by the function factor).

The default is given by mclust.options("classPlotColors").

. . . further arguments passed to or from other methods.

plot.MclustDA 117

Details

For more flexibility in plotting, use mclust1Dplot, mclust2Dplot, surfacePlot, coordProj, or randProj.

References

C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611-631*.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

Author(s)

Luca Scrucca

See Also

MclustDA, surfacePlot, coordProj, randProj

```
## Not run:
odd \leftarrow seq(from = 1, to = nrow(iris), by = 2)
even <- odd + 1
X.train <- iris[odd,-5]</pre>
Class.train <- iris[odd,5]</pre>
X.test <- iris[even,-5]</pre>
Class.test <- iris[even,5]</pre>
# common EEE covariance structure (which is essentially equivalent to linear discriminant analysis)
irisMclustDA <- MclustDA(X.train, Class.train, modelType = "EDDA", modelNames = "EEE")</pre>
summary(irisMclustDA, parameters = TRUE)
summary(irisMclustDA, newdata = X.test, newclass = Class.test)
# common covariance structure selected by BIC
irisMclustDA <- MclustDA(X.train, Class.train, modelType = "EDDA")</pre>
summary(irisMclustDA, parameters = TRUE)
summary(irisMclustDA, newdata = X.test, newclass = Class.test)
# general covariance structure selected by BIC
irisMclustDA <- MclustDA(X.train, Class.train)</pre>
summary(irisMclustDA, parameters = TRUE)
summary(irisMclustDA, newdata = X.test, newclass = Class.test)
plot(irisMclustDA)
plot(irisMclustDA, dimens = 3:4)
plot(irisMclustDA, dimens = 4)
plot(irisMclustDA, what = "classification")
plot(irisMclustDA, what = "classification", newdata = X.test)
```

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```
plot(irisMclustDA, what = "classification", dimens = 3:4)
plot(irisMclustDA, what = "classification", newdata = X.test, dimens = 3:4)
plot(irisMclustDA, what = "classification", dimens = 4)
plot(irisMclustDA, what = "classification", dimens = 4, newdata = X.test)
plot(irisMclustDA, what = "train&test", newdata = X.test)
plot(irisMclustDA, what = "train&test", newdata = X.test, dimens = 3:4)
plot(irisMclustDA, what = "train&test", newdata = X.test, dimens = 4)
plot(irisMclustDA, what = "error")
plot(irisMclustDA, what = "error", dimens = 3:4)
plot(irisMclustDA, what = "error", dimens = 4)
plot(irisMclustDA, what = "error", newdata = X.test, newclass = Class.test)
plot(irisMclustDA, what = "error", newdata = X.test, newclass = Class.test, dimens = 3:4)
plot(irisMclustDA, what = "error", newdata = X.test, newclass = Class.test, dimens = 4)
# simulated 1D data
n <- 250
set.seed(1)
triModal \leftarrow c(rnorm(n,-5), rnorm(n,0), rnorm(n,5))
triClass \leftarrow c(rep(1,n), rep(2,n), rep(3,n))
odd <- seq(from = 1, to = length(triModal), by = 2)
even <- odd + 1
triMclustDA <- MclustDA(triModal[odd], triClass[odd])</pre>
summary(triMclustDA, parameters = TRUE)
summary(triMclustDA, newdata = triModal[even], newclass = triClass[even])
plot(triMclustDA)
plot(triMclustDA, what = "classification")
plot(triMclustDA, what = "classification", newdata = triModal[even])
plot(triMclustDA, what = "train&test", newdata = triModal[even])
plot(triMclustDA, what = "error")
plot(triMclustDA, what = "error", newdata = triModal[even], newclass = triClass[even])
# simulated 2D cross data
data(cross)
odd \leftarrow seq(from = 1, to = nrow(cross), by = 2)
even \leftarrow odd + 1
crossMclustDA <- MclustDA(cross[odd,-1], cross[odd,1])</pre>
summary(crossMclustDA, parameters = TRUE)
summary(crossMclustDA, newdata = cross[even,-1], newclass = cross[even,1])
plot(crossMclustDA)
plot(crossMclustDA, what = "classification")
plot(crossMclustDA, what = "classification", newdata = cross[even,-1])
plot(crossMclustDA, what = "train&test", newdata = cross[even,-1])
plot(crossMclustDA, what = "error")
plot(crossMclustDA, what = "error", newdata =cross[even,-1], newclass = cross[even,1])
## End(Not run)
```

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plot.MclustDR

Plotting method for dimension reduction for model-based clustering and classification

Description

Graphs data projected onto the estimated subspace for model-based clustering and classification.

Usage

```
## S3 method for class 'MclustDR'
plot(x, dimens,
     what = c("scatterplot", "pairs", "contour", "classification",
              "boundaries", "density", "evalues"),
     symbols, colors, col.contour = gray(0.7), col.sep = grey(0.4),
     ngrid = 100, nlevels = 5, asp = NULL, ...)
```

Arguments Χ

An object of class 'MclustDR' resulting from a call to MclustDR.

dimens

A vector of integers giving the dimensions of the desired coordinate projections for multivariate data.

what

The type of graph requested:

- "scatterplot" = a two-dimensional plot of data projected onto the first two directions specified by dimens and with data points marked according to the corresponding mixture component. By default, the first two directions are selected for plotting.
- "pairs" = a scatterplot matrix of data projected onto the estimated subspace and with data points marked according to the corresponding mixture component. By default, all the available directions are used, unless they have been specified by dimens.
- "contour" = a two-dimensional plot of data projected onto the first two directions specified by dimens (by default, the first two directions) with density contours for classes or clusters and data points marked according to the corresponding mixture component.
- "classification" = a two-dimensional plot of data projected onto the first two directions specified by dimens (by default, the first two directions) with classification region and data points marked according to the corresponding mixture component.
- "boundaries" = a two-dimensional plot of data projected onto the first two directions specified by dimens (by default, the first two directions) with uncertainty boundaries and data points marked according to the corresponding mixture component. The uncertainty is shown using a greyscale with darker regions indicating higher uncertainty.
- "density" = a one-dimensional plot of estimated density for the first direction specified by dimens (by default, the first one). A set of box-plots for each estimated cluster or known class are also shown at the bottom of the graph.

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symbols	Either an integer or character vector assigning a plotting symbol to each unique mixture component. Elements in colors correspond to classes in order of appearance in the sequence of observations (the order used by the function factor). The default is given by mclust.options("classPlotSymbols").
colors	Either an integer or character vector assigning a color to each unique cluster or known class. Elements in colors correspond to classes in order of appearance in the sequence of observations (the order used by the function factor). The default is given by mclust.options("classPlotColors").
col.contour	The color of contours in case what = "contour".
col.sep	The color of classification boundaries in case what = "classification".
ngrid	An integer specifying the number of grid points to use in evaluating the classification regions.
nlevels	
	The number of levels to use in case what = "contour".
asp	The number of levels to use in case what = "contour". For scatterplots the y/x aspect ratio, see plot.window.

Author(s)

Luca Scrucca

References

Scrucca, L. (2010) Dimension reduction for model-based clustering. *Statistics and Computing*, 20(4), pp. 471-484.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

MclustDR

```
mod = Mclust(iris[,1:4], G = 3)
dr = MclustDR(mod)
plot(dr, what = "evalues")
plot(dr, what = "pairs")
plot(dr, what = "scatterplot", dimens = c(1,3))
plot(dr, what = "contour")
plot(dr, what = "classification", ngrid = 200)
plot(dr, what = "boundaries", ngrid = 200)
plot(dr, what = "density")
plot(dr, what = "density")
plot(dr, what = "density", dimens = 2)

data(banknote)
da = MclustDA(banknote[,2:7], banknote$Status, G = 1:3)
dr = MclustDR(da)
```

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```
plot(dr, what = "evalues")
plot(dr, what = "pairs")
plot(dr, what = "contour")
plot(dr, what = "contour", dimens = c(1,3))
plot(dr, what = "classification", ngrid = 200)
plot(dr, what = "boundaries", ngrid = 200)
plot(dr, what = "density")
plot(dr, what = "density", dimens = 2)
```

plot.mclustICL

ICL Plot for Model-Based Clustering

Description

Plots the ICL values returned by the mclustICL function.

Usage

```
## S3 method for class 'mclustICL'
plot(x, ylab = "ICL", ...)
```

Arguments

```
    x Output from mclustICL.
    ylab Label for the vertical axis of the plot.
    ... Further arguments passed to the plot.mclustBIC function.
```

Value

A plot of the ICL values.

References

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

```
mclustICL
```

```
## Not run:
data(faithful)
faithful.ICL = mclustICL(faithful)
plot(faithful.ICL)
## End(Not run)
```

122 predict.densityMclust

predict.densityMclust Density estimate of multivariate observations by Gaussian finite mixture modeling

Description

Compute density estimation for multivariate observations based on Gaussian finite mixture models estimated by densityMclust.

Usage

```
## S3 method for class 'densityMclust'
predict(object, newdata, what = c("dens", "cdens"), ...)
```

Arguments

object an object of class 'densityMclust' resulting from a call to densityMclust.

newdata a vector, a data frame or matrix giving the data. If missing the density is computed for the input data obtained from the call to densityMclust.

what a character string specifying what to retrieve: "dens" returns a vector of values for the mixture density, cdens returns a matrix of component densities for each mixture component (along the columns).

... further arguments passed to or from other methods.

Value

Returns a vector or a matrix of densities evaluated at newdata depending on the argument what (see above).

Author(s)

Luca Scrucca

References

- C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association* 97:611:631.
- C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

Mclust.

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Examples

```
x = faithful$waiting
dens = densityMclust(x)
x0 = seq(50, 100, by = 10)
d0 = predict(dens, x0)
plot(dens)
points(x0, d0, pch = 20)
```

predict.Mclust

Cluster multivariate observations by Gaussian finite mixture modeling

Description

Cluster prediction for multivariate observations based on Gaussian finite mixture models estimated by Mclust.

Usage

```
## S3 method for class 'Mclust'
predict(object, newdata, ...)
```

Arguments

object an object of class 'Mclust' resulting from a call to Mclust.

newdata a data frame or matrix giving the data. If missing the clustering data obtained

from the call to Mclust are classified.

... further arguments passed to or from other methods.

Value

Returns a list of with the following components:

classification a factor of predicted cluster labels for newdata.

a matrix whose [i,k]th entry is the probability that observation i in newdata belongs to the kth cluster.

Author(s)

Luca Scrucca

- C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611:631*.
- C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

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See Also

Mclust.

Examples

```
model <- Mclust(faithful)

# predict cluster for the observed data
pred <- predict(model)
str(pred)
pred$z  # equal to model$z
pred$classification # equal to
plot(faithful, col = pred$classification, pch = pred$classification)

# predict cluster over a grid
grid <- apply(faithful, 2, function(x) seq(min(x), max(x), length = 50))
grid <- expand.grid(eruptions = grid[,1], waiting = grid[,2])
pred <- predict(model, grid)
plot(grid, col = mclust.options("classPlotColors")[pred$classification], pch = 15, cex = 0.5)
points(faithful, pch = model$classification)</pre>
```

predict.MclustDA Classify multivariate observations by Gaussian finite mixture modeling

Description

Classify multivariate observations based on Gaussian finite mixture models estimated by MclustDA.

Usage

```
## S3 method for class 'MclustDA'
predict(object, newdata, prior, ...)
```

Arguments

object	an object of class 'MclustDA' resulting from a call to MclustDA.
newdata	a data frame or matrix giving the data. If missing the train data obtained from the call to MclustDA are classified.
prior	the prior probabilities of the classes; by default, this is set at the proportions in the training data.
	further arguments passed to or from other methods.

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Value

Returns a list of with the following components:

classification a factor of predicted class labels for newdata.

z a matrix whose [i,k]th entry is the probability that observation i in newdata belongs to the kth class.

Author(s)

Luca Scrucca

References

C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611:631*.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

MclustDA.

```
## Not run:
odd <- seq(from = 1, to = nrow(iris), by = 2)
even <- odd + 1
X.train <- iris[odd,-5]
Class.train <- iris[odd,5]
X.test <- iris[even,-5]
Class.test <- iris[even,5]
irisMclustDA <- MclustDA(X.train, Class.train)
predTrain <- predict(irisMclustDA)
predTrain
predTest <- predict(irisMclustDA, X.test)
predTest
## End(Not run)</pre>
```

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predict.MclustDR	Classify multivariate observations on a dimension reduced subspace by Gaussian finite mixture modeling

Description

Classify multivariate observations on a dimension reduced subspace estimated from a Gaussian finite mixture model.

Usage

```
## S3 method for class 'MclustDR'
predict(object, dim = 1:object$numdir, newdata, eval.points, ...)
```

Arguments

an object of class 'MclustDR' resulting from a call to MclustDR. object dim the dimensions of the reduced subspace used for prediction. a data frame or matrix giving the data. If missing the data obtained from the call newdata to MclustDR are used. a data frame or matrix giving the data projected on the reduced subspace. If eval.points provided newdata is not used. further arguments passed to or from other methods.

Value

Returns a list of with the following components:

dir a matrix containing the data projected onto the dim dimensions of the reduced

subspace.

density densities from mixture model for each data point.

a matrix whose [i,k]th entry is the probability that observation i in newdata

belongs to the kth class.

uncertainty The uncertainty associated with the classification. classification A vector of values giving the MAP classification.

Author(s)

Luca Scrucca

References

Scrucca, L. (2010) Dimension reduction for model-based clustering. Statistics and Computing, 20(4), pp. 471-484.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

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See Also

MclustDR.

Examples

```
mod = Mclust(iris[,1:4])
dr = MclustDR(mod)
pred = predict(dr)
str(pred)

data(banknote)
mod = MclustDA(banknote[,2:7], banknote$Status)
dr = MclustDR(mod)
pred = predict(dr)
str(pred)
```

print.clustCombi

Displays Combined Clusterings Results

Description

Displays the Gaussian mixture model and number of components selected by Mclust/BIC and the components proportions and means of the fitted corresponding distribution. Then, informations about the combining steps.

Usage

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

Arguments

x An object of class 'clustCombi'. Typically an output from the clustCombi function.

... additional arguments.

Author(s)

J.-P. Baudry, A. E. Raftery, L. Scrucca

References

J.-P. Baudry, A. E. Raftery, G. Celeux, K. Lo and R. Gottardo (2010). Combining mixture components for clustering. *Journal of Computational and Graphical Statistics*, 19(2):332-353.

See Also

clustCombi

128 priorControl

Examples

```
## Not run:
data(Baudry_etal_2010_JCGS_examples)
## 2D Example
output <- clustCombi(ex4.1)
output
## End(Not run)</pre>
```

priorControl

Conjugate Prior for Gaussian Mixtures.

Description

Specify a conjugate prior for Gaussian mixtures.

Usage

```
priorControl(functionName = "defaultPrior", ...)
```

Arguments

functionName

The name of the function specifying the conjugate prior. By default the function defaultPrior is used, and this can also be used as a template for alternative specification.

• • •

Optional named arguments to the function specified in functionName together with their values.

Details

The function priorControl is used to specify a conjugate prior for EM within *MCLUST*. Note that, as described in defaultPrior, in the multivariate case only 10 out of 14 models may be used in conjunction with a prior, i.e. those available in *MCLUST* up to version 4.4.

Value

A list with the function name as the first component. The remaining components (if any) consist of a list of arguments to the function with assigned values.

- C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611-631*.
- C. Fraley and A. E. Raftery (2005). Bayesian regularization for normal mixture estimation and model-based clustering. Technical Report, Department of Statistics, University of Washington.

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C. Fraley and A. E. Raftery (2007). Bayesian regularization for normal mixture estimation and model-based clustering. *Journal of Classification* 24:155-181.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

```
mclustBIC, me, mstep, defaultPrior
```

Examples

```
# default prior
irisBIC <- mclustBIC(iris[,-5], prior = priorControl())
summary(irisBIC, iris[,-5])
# no prior on the mean; default prior on variance
irisBIC <- mclustBIC(iris[,-5], prior = priorControl(shrinkage = 0))
summary(irisBIC, iris[,-5])</pre>
```

randomPairs

Random hierarchical structure

Description

Create a hierarchical structure using a random partition of the data.

Usage

```
randomPairs(data, seed, ...)
```

Arguments

data	A numeric matrix or data frame of observations. If a matrix or data frame, rows
	correspond to observations and columns correspond to variables.
seed	Optional single value, interpreted as an integer, specifying the seed for random partition.
	Catches unused arguments in indirect or list calls via do.call.

Value

A numeric two-column matrix in which the *i*th row gives the minimum index for observations in each of the two clusters merged at the *i*th stage of a random agglomerative hierarchical clustering.

References

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

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See Also

```
hc, hclass hcVVV
```

Examples

```
data <- iris[,1:4]
randPairs <- randomPairs(data)
str(randPairs)
# start model-based clustering from a random partition
mod <- Mclust(data, initialization = list(hcPairs = randPairs))
summary(mod)</pre>
```

randProj

Random projections of multidimensional data modeled by an MVN mixture.

Description

Plots random projections given multidimensional data and parameters of an MVN mixture model for the data.

Usage

Arguments

data A numeric matrix or data frame of observations. Categorical variables are not

allowed. If a matrix or data frame, rows correspond to observations and columns

correspond to variables.

mixture model.

seeds A vector if integer seeds for random number generation. Elements should be in

the range 0:1000. Each seed should produce a different projection.

parameters A named list giving the parameters of an *MCLUST* model, used to produce superimposing ellipses on the plot. The relevant components are as follows:

mean The mean for each component. If there is more than one component, this is a matrix whose kth column is the mean of the *k*th component of the

variance A list of variance parameters for the model. The components of this list depend on the model specification. See the help file for mclustVariance for details.

A matrix in which the [i,k]th entry gives the probability of observation i belonging to the kth class. Used to compute classification and uncertainty if those arguments aren't available.

z

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classification	A numeric or character vector representing a classification of observations (rows) of data. If present argument z will be ignored.
truth	A numeric or character vector giving a known classification of each data point. If classification or z is also present, this is used for displaying classification errors.
uncertainty	A numeric vector of values in $(0,1)$ giving the uncertainty of each data point. If present argument z will be ignored.
what	Choose from one of the following three options: "classification" (default), "errors", "uncertainty".
quantiles	A vector of length 2 giving quantiles used in plotting uncertainty. The smallest symbols correspond to the smallest quantile (lowest uncertainty), medium-sized (open) symbols to points falling between the given quantiles, and large (filled) symbols to those in the largest quantile (highest uncertainty). The default is $(0.75,0.95)$.
symbols	Either an integer or character vector assigning a plotting symbol to each unique class in classification. Elements in colors correspond to classes in order of appearance in the sequence of observations (the order used by the function unique). The default is given by mclust.options("classPlotSymbols").
colors	Either an integer or character vector assigning a color to each unique class in classification. Elements in colors correspond to classes in order of appearance in the sequence of observations (the order used by the function unique). The default is given by mclust.options("classPlotColors").
scale	A logical variable indicating whether or not the two chosen dimensions should be plotted on the same scale, and thus preserve the shape of the distribution. Default: scale=FALSE
xlim, ylim	Arguments specifying bounds for the ordinate, abscissa of the plot. This may be useful for when comparing plots.
CEX	An argument specifying the size of the plotting symbols. The default value is 1.
PCH	An argument specifying the symbol to be used when a classification has not been specified for the data. The default value is a small dot ".".
main	A logical variable or NULL indicating whether or not to add a title to the plot identifying the dimensions used.
	Other graphics parameters.

Side Effects

A plot showing a random two-dimensional projection of the data, together with the location of the mixture components, classification, uncertainty, and/or classification errors.

References

C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611-631*.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

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See Also

```
clPairs, coordProj, mclust2Dplot, mclust.options
```

Examples

sigma2decomp

Convert mixture component covariances to decomposition form.

Description

Converts a set of covariance matrices from representation as a 3-D array to a parameterization by eigenvalue decomposition.

Usage

```
sigma2decomp(sigma, G = NULL, tol = sqrt(.Machine$double.eps), ...)
```

Arguments

sigma	Either a 3-D array whose [,,k]th component is the covariance matrix for the kth component in an MVN mixture model, or a single covariance matrix in the case that all components have the same covariance.
G	The number of components in the mixture. When sigma is a 3-D array, the number of components can be inferred from its dimensions.
tol	Tolerance for determining whether or not the covariances have equal volume, shape, and or orientation. The default is the square root of the relative machine precision, sqrt(.Machine\$double.eps), which is about 1.e-8.
	Catches unused arguments from an indirect or list call via do.call.

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Value

The covariance matrices for the mixture components in decomposition form, including the following components:

modelName	A character string indicating the infered model. The help file for mclustModelNames
-----------	---

describes the available models.

d The dimension of the data.

G The number of components in the mixture model.

scale Either a G-vector giving the scale of the covariance (the dth root of its determi-

nant) for each component in the mixture model, or a single numeric value if the

scale is the same for each component.

shape Either a G by d matrix in which the kth column is the shape of the covariance

matrix (normalized to have determinant 1) for the kth component, or a d-vector

giving a common shape for all components.

orientation Either a d by d by G array whose [,,k]th entry is the orthonomal matrix whose

columns are the eigenvectors of the covariance matrix of the kth component, or a d by d orthonormal matrix if the mixture components have a common orientation. The orientation component of decomp can be omitted in spherical and diagonal models, for which the principal components are parallel to the coordi-

nate axes so that the orientation matrix is the identity.

References

C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association* 97:611-631.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

decomp2sigma

```
meEst <- meEEE(iris[,-5], unmap(iris[,5]))
names(meEst$parameters$variance)
meEst$parameters$variance$Sigma
sigma2decomp(meEst$parameters$variance$Sigma, G = length(unique(iris[,5])))</pre>
```

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sim

Simulate from Parameterized MVN Mixture Models

Description

Simulate data from parameterized MVN mixture models.

Usage

```
sim(modelName, parameters, n, seed = NULL, ...)
```

Arguments

modelName A character string indicating the model. The help file for mclustModelNames

describes the available models.

parameters A list with the following components:

pro A vector whose *k*th component is the mixing proportion for the *k*th component of the mixture model. If missing, equal proportions are assumed.

mean The mean for each component. If there is more than one component, this is a matrix whose kth column is the mean of the *k*th component of the mixture model

variance A list of variance parameters for the model. The components of this list depend on the model specification. See the help file for mclustVariance for details.

n An integer specifying the number of data points to be simulated.

seed An optional integer argument to set.seed for reproducible random class as-

signment. By default the current seed will be used. Reproducibility can also be

achieved by calling set.seed before calling sim.

... Catches unused arguments in indirect or list calls via do.call.

Details

This function can be used with an indirect or list call using do.call, allowing the output of e.g. mstep, em, me, Mclust to be passed directly without the need to specify individual parameters as arguments.

Value

A matrix in which first column is the classification and the remaining columns are the n observations simulated from the specified MVN mixture model.

Attributes: "modelName" A character string indicating the variance model used for the sim-

ulation.

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References

C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611-631*.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

```
simE, ..., simVVV, Mclust, mstep, do.call
```

```
irisBIC <- mclustBIC(iris[,-5])</pre>
irisModel <- mclustModel(iris[,-5], irisBIC)</pre>
names(irisModel)
irisSim <- sim(modelName = irisModel$modelName,</pre>
                parameters = irisModel$parameters,
                n = nrow(iris))
## Not run:
  do.call("sim", irisModel) # alternative call
## End(Not run)
par(pty = "s", mfrow = c(1,2))
dimnames(irisSim) <- list(NULL, c("dummy", (dimnames(iris)[[2]])[-5]))</pre>
dimens \leftarrow c(1,2)
lim1 <- apply(iris[,dimens],2,range)</pre>
lim2 <- apply(irisSim[,dimens+1],2,range)</pre>
lims <- apply(rbind(lim1,lim2),2,range)</pre>
xlim <- lims[,1]</pre>
ylim <- lims[,2]</pre>
coordProj(iris[,-5], parameters=irisModel$parameters,
           classification=map(irisModel$z),
           dimens=dimens, xlim=xlim, ylim=ylim)
coordProj(iris[,-5], parameters=irisModel$parameters,
           classification=map(irisModel$z), truth = irisSim[,-1],
           dimens=dimens, xlim=xlim, ylim=ylim)
irisModel3 <- mclustModel(iris[,-5], irisBIC, G=3)</pre>
irisSim3 <- sim(modelName = irisModel3$modelName,</pre>
                parameters = irisModel3$parameters, n = 500, seed = 1)
## Not run:
 irisModel3$n <- NULL
 irisSim3 <- do.call("sim",c(list(n=500,seed=1),irisModel3)) # alternative call</pre>
```

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```
## End(Not run)
clPairs(irisSim3[,-1], cl = irisSim3[,1])
```

simE

Simulate from a Parameterized MVN Mixture Model

Description

Simulate data from a parameterized MVN mixture model.

Usage

```
simE(parameters, n, seed = NULL, ...)
simV(parameters, n, seed = NULL, ...)
simEII(parameters, n, seed = NULL, ...)
simVII(parameters, n, seed = NULL, ...)
simEEI(parameters, n, seed = NULL, ...)
simVEI(parameters, n, seed = NULL, ...)
simEVI(parameters, n, seed = NULL, ...)
simVVI(parameters, n, seed = NULL, ...)
simEEE(parameters, n, seed = NULL, ...)
simEEV(parameters, n, seed = NULL, ...)
simVEV(parameters, n, seed = NULL, ...)
simVVV(parameters, n, seed = NULL, ...)
simEVE(parameters, n, seed = NULL, ...)
simEVV(parameters, n, seed = NULL, ...)
simVEE(parameters, n, seed = NULL, ...)
simVVE(parameters, n, seed = NULL, ...)
```

Arguments

n

seed

parameters

A list with the following components:

pro A vector whose *k*th component is the mixing proportion for the *k*th component of the mixture model. If missing, equal proportions are assumed.

mean The mean for each component. If there is more than one component, this is a matrix whose kth column is the mean of the *k*th component of the mixture model.

variance A list of variance parameters for the model. The components of this list depend on the model specification. See the help file for mclustVariance for details.

An integer specifying the number of data points to be simulated.

An optional integer argument to set.seed for reproducible random class assignment. By default the current seed will be used. Reproducibility can also be

achieved by calling set. seed before calling sim.

.. Catches unused arguments in indirect or list calls via do. call.

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Details

This function can be used with an indirect or list call using do.call, allowing the output of e.g. mstep, em me, Mclust, to be passed directly without the need to specify individual parameters as arguments.

Value

A matrix in which first column is the classification and the remaining columns are the n observations simulated from the specified MVN mixture model.

Attributes: "modelName" A character string indicating the variance model used for the simulation.

References

C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611-631*.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

sim, Mclust, mstepE, mclustVariance.

```
d <- 2
G <- 2
scale <- 1
shape \leftarrow c(1, 9)
01 < - diag(2)
02 \leftarrow diag(2)[,c(2,1)]
0 <- array(cbind(01,02), c(2, 2, 2))</pre>
variance <- list(d= d, G = G, scale = scale, shape = shape, orientation = 0)</pre>
mu <- matrix(0, d, G) ## center at the origin
simdat <- simEEV( n = 200,
                   parameters = list(pro=c(1,1),mean=mu,variance=variance),
                   seed = NULL)
cl <- simdat[,1]</pre>
## Not run:
sigma <- array(apply(0, 3, function(x,y) crossprod(x*y),</pre>
                  y = sqrt(scale*shape)), c(2,2,2))
paramList <- list(mu = mu, sigma = sigma)</pre>
coordProj( simdat, paramList = paramList, classification = cl)
```

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```
## End(Not run)
```

summary.Mclust

Summarizing Gaussian Finite Mixture Model Fits

Description

Summary method for class "Mclust".

Usage

```
## S3 method for class 'Mclust'
summary(object, parameters = FALSE, classification = FALSE, ...)
## S3 method for class 'summary.Mclust'
print(x, digits = getOption("digits"), ...)
```

Arguments

object An object of class 'Mclust' resulting of a call to Mclust or densityMclust.

x An object of class 'summary.Mclust', usually, a result of a call to summary.Mclust.

parameters Logical; if TRUE, the parameters of mixture components are printed.

classification Logical; if TRUE, the MAP classification/clustering of observations is printed.

digits The number of significant digits to use when printing.
... Further arguments passed to or from other methods.

Author(s)

Luca Scrucca

References

- C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611:631*.
- C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

Mclust, densityMclust.

summary.mclustBIC 139

Examples

```
mod1 = Mclust(iris[,1:4])
summary(mod1)
summary(mod1, parameters = TRUE, classification = TRUE)

mod2 = Mclust(iris[,1:4], G = 1)
summary(mod2, parameters = TRUE, classification = TRUE)

mod3 = Mclust(iris[,1:4], prior = priorControl())
summary(mod3)

mod4 = Mclust(iris[,1:4], prior = priorControl(functionName="defaultPrior", shrinkage=0.1))
summary(mod4, parameters = TRUE, classification = TRUE)
```

summary.mclustBIC

Summary function for model-based clustering via BIC

Description

Optimal model characteristics and classification for model-based clustering via mclustBIC.

Usage

```
## S3 method for class 'mclustBIC'
summary(object, data, G, modelNames, ...)
```

Arguments

object An 'mclustBIC' object, which is the result of applying mclustBIC to data.

data The matrix or vector of observations used to generate 'object'.

G A vector of integers giving the numbers of mixture components (clusters) from

which the best model according to BIC will be selected (as.character(G) must be a subset of the row names of object). The default is to select the best model

for all numbers of mixture components used to obtain object.

modelNames A vector of integers giving the model parameterizations from which the best

model according to BIC will be selected (as.character(model) must be a subset of the column names of object). The default is to select the best model for

parameterizations used to obtain object.

... Not used. For generic/method consistency.

Value

A list giving the optimal (according to BIC) parameters, conditional probabilities z, and log-likelihood, together with the associated classification and its uncertainty.

The details of the output components are as follows:

modelName A character string denoting the model corresponding to the optimal BIC.

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n The number of observations in the data.

d The dimension of the data.

G The number of mixture components in the model corresponding to the optimal

BIC.

bic The optimal BIC value.

loglik The log-likelihood corresponding to the optimal BIC.

parameters A list with the following components:

pro A vector whose *k*th component is the mixing proportion for the *k*th component of the mixture model. If missing, equal proportions are assumed.

mean The mean for each component. If there is more than one component, this is a matrix whose kth column is the mean of the *k*th component of the mixture model.

variance A list of variance parameters for the model. The components of this list depend on the model specification. See the help file for mclustVariance for details.

z A matrix whose [i,k]th entry is the probability that observation i in the data

belongs to the kth class.

classification map(z): The classification corresponding to z.

uncertainty The uncertainty associated with the classification.

Attributes: "bestBICvalues" Some of the best bic values for the analysis.

"prior" The prior as specified in the input.

"control" The control parameters for EM as specified in the input.

"initialization" The parameters used to initial EM for computing the maxi-

mum likelihood values used to obtain the BIC.

References

C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611-631*.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

```
mclustBIC mclustModel
```

```
irisBIC <- mclustBIC(iris[,-5])
summary(irisBIC, iris[,-5])
summary(irisBIC, iris[,-5], G = 1:6, modelNames = c("VII", "VVI", "VVV"))</pre>
```

```
summary.MclustBootstrap
```

Summary Function for Bootstrap Inference for Gaussian Finite Mixture Models

Description

Summary of bootstrap distribution for the parameters of a Gaussian mixture model providing either standard errors or percentile bootstrap confidence intervals.

Usage

```
## S3 method for class 'MclustBootstrap'
summary(object, what = c("se", "ci"), conf.level = 0.95, ...)
```

Arguments

object	An object of class 'MclustBootstrap' as returned by MclustBootstrap.
what	A character string: "se" for the standard errors; "ci" for the confidence intervals.
conf.level	A value specifying the confidence level of the interval.
	Further arguments passed to or from other methods.

Details

For details about the procedure used to obtain the bootstrap distribution see MclustBootstrap.

References

Davison, A. and Hinkley, D. (1997) *Bootstrap Methods and Their Applications*. Cambridge University Press.

McLachlan, G.J. and Peel, D. (2000) Finite Mixture Models. Wiley.

See Also

MclustBootstrap.

```
## Not run:
data(diabetes)
X = diabetes[,-1]
modClust = Mclust(X)
bootClust = MclustBootstrap(modClust)
summary(bootClust, what = "se")
summary(bootClust, what = "ci")
```

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```
data(acidity)
modDens = densityMclust(acidity)
modDens = MclustBootstrap(modDens)
summary(modDens, what = "se")
summary(modDens, what = "ci")
## End(Not run)
```

summary.MclustDA

Summarizing discriminant analysis based on Gaussian finite mixture modeling.

Description

Summary method for class "MclustDA".

Usage

```
## S3 method for class 'MclustDA'
summary(object, parameters = FALSE, newdata, newclass, ...)
## S3 method for class 'summary.MclustDA'
print(x, digits = getOption("digits"), ...)
```

Arguments

object	An object of class 'MclustDA' resulting from a call to MclustDA.
x	An object of class 'summary.MclustDA', usually, a result of a call to summary.MclustDA.
parameters	Logical; if TRUE, the parameters of mixture components are printed.
newdata	A data frame or matrix giving the test data.
newclass	A vector giving the class labels for the observations in the test data.
digits	The number of significant digits to use when printing.
	Further arguments passed to or from other methods.

Value

The function summary. MclustDA computes and returns a list of summary statistics of the estimated MclustDA or EDDA model for classification.

Author(s)

Luca Scrucca

summary.MclustDR 143

References

C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611:631*.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

See Also

```
MclustDA, plot.MclustDA.
```

Examples

```
mod = MclustDA(data = iris[,1:4], class = iris$Species)
summary(mod)
summary(mod, parameters = TRUE)
```

summary.MclustDR

Summarizing dimension reduction method for model-based clustering and classification

Description

Summary method for class "MclustDR".

Usage

```
## S3 method for class 'MclustDR'
summary(object, numdir, std = FALSE, ...)
## S3 method for class 'summary.MclustDR'
print(x, digits = max(5, getOption("digits") - 3), ...)
```

Arguments

object	An object of class 'MclustDR' resulting from a call to MclustDR.
x	$An \ object \ of \ class \ 's ummary. \ MclustDR', usually, a \ result \ of \ a \ call \ to \ summary. \ MclustDR.$
numdir	An integer providing the number of basis directions to be printed.
std	if TRUE the coefficients basis are scaled such that all predictors have unit standard deviation.
digits	The number of significant digits to use when printing.
	Further arguments passed to or from other methods.

Author(s)

Luca Scrucca

144 surfacePlot

References

Scrucca, L. (2010) Dimension reduction for model-based clustering. *Statistics and Computing*, 20(4), pp. 471-484.

See Also

```
MclustDR, plot.MclustDR
```

surfacePlot

Density or uncertainty surface for bivariate mixtures.

Description

Plots a density or uncertainty surface given bivariate data and parameters of an MVN mixture model for the data.

Usage

Arguments

data

A matrix, or data frame of bivariate observations. Categorical variables are not allowed. If a matrix or data frame, rows correspond to observations and columns correspond to variables.

parameters

A named list giving the parameters of an *MCLUST* model, used to produce superimposing ellipses on the plot. The relevant components are as follows:

mean The mean for each component. If there is more than one component, this is a matrix whose kth column is the mean of the *k*th component of the mixture model.

variance A list of variance parameters for the model. The components of this list depend on the model specification. See the help file for mclustVariance for details.

type

Choose from one of the following three options: "contour" (default), "image", "persp" indicating the plot type.

what

Choose from one of the following options: "density" (default), "uncertainty" indicating what to plot.

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transformation	Choose from one of the following three options: "none" (default), "log", "sqrt" indicating a transformation to be applied before plotting.
grid	The number of grid points (evenly spaced on each axis). The mixture density and uncertainty is computed at grid x grid points to produce the surface plot. Default: 100.
nlevels	The number of levels to use for a contour plot. Default: 11.
levels	A vector of levels at which to draw the lines in a contour plot.
col	The color to be used for drawing contour lines.
xlim, ylim	Optional argument specifying bounds for the ordinate, abscissa of the plot. This may be useful for when comparing plots.
xlab, ylab	Optional argument specifying labels for the x-axis and y-axis.
scale	A logical variable indicating whether or not the two dimensions should be plotted on the same scale, and thus preserve the shape of the distribution. The default is not to scale.
main	A logical variable or NULL indicating whether or not to add a title to the plot identifying the dimensions used.
swapAxes	A logical variable indicating whether or not the axes should be swapped for the plot.
verbose	A logical variable telling whether or not to print an indication that the function is in the process of computing values at the grid points, which typically takes some time to complete.
	Other graphics parameters.

Value

An invisible list with components x, y, and z in which x and y are the values used to define the grid and z is the transformed density or uncertainty at the grid points.

Side Effects

A plots showing (a transformation of) the density or uncertainty for the given mixture model and data.

Details

For an image plot, a color scheme may need to be selected on the display device in order to view the plot.

References

C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611-631*.

C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

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See Also

```
mclust2Dplot
```

Examples

thyroid

Thyroid gland data

Description

Data on five laboratory tests administered to a sample of 215 patients. The tests are used to predict whether a patient's thyroid can be classified as euthyroidism (normal thyroid gland function), hypothyroidism (underactive thyroid not producing enough thyroid hormone) or hyperthyroidism (overactive thyroid producing and secreting excessive amounts of the free thyroid hormones T3 and/or thyroxine T4). Diagnosis of thyroid operation was based on a complete medical record, including anamnesis, scan, etc..

Usage

```
data(thyroid)
```

Format

A data frame with the following variables:

Diagnosis Diagnosis of thyroid operation: Hypo, Normal, and Hyper.

RT3U T3-resin uptake test (percentage).

T4 Total Serum thyroxin as measured by the isotopic displacement method.

T3 Total serum triiodothyronine as measured by radioimmuno assay.

TSH Basal thyroid-stimulating hormone (TSH) as measured by radioimmuno assay.

DTSH Maximal absolute difference of TSH value after injection of 200 micro grams of thyrotropin-releasing hormone as compared to the basal value.

Source

UCI ftp://ftp.ics.uci.edu/pub/machine-learning-databases/thyroid-disease/

uncerPlot 147

References

Coomans, D., Broeckaert, M. Jonckheer M. and Massart D.L. (1983) Comparison of Multivariate Discriminant Techniques for Clinical Data - Application to the Thyroid Functional State, *Meth. Inform. Med.* 22, pp. 93-101.

Coomans, D. and I. Broeckaert (1986) *Potential Pattern Recognition in Cemical and Medical Decision Making*, Research Studies Press, Letchworth, England.

uncerPlot

Uncertainty Plot for Model-Based Clustering

Description

Displays the uncertainty in converting a conditional probability from EM to a classification in model-based clustering.

Usage

```
uncerPlot(z, truth, ...)
```

Arguments

z A matrix whose [i,k]th entry is the conditional probability of the ith observation belonging to the kth component of the mixture.

truth A numeric or character vector giving the true classification of the data.

Provided to allow lists with elements other than the arguments can be passed in indirect or list calls with do.call.

Details

When truth is provided and the number of classes is compatible with z, the function compareClass is used to to find best correspondence between classes in truth and z.

Value

A plot of the uncertainty profile of the data, with uncertainties in increasing order of magnitude. If truth is supplied and the number of classes is the same as the number of columns of z, the uncertainty of the misclassified data is marked by vertical lines on the plot.

- C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611-631*.
- C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

148 unmap

See Also

```
mclustBIC, em, me, mapClass
```

Examples

```
irisModel3 <- Mclust(iris[,-5], G = 3)
uncerPlot(z = irisModel3$z)
uncerPlot(z = irisModel3$z, truth = iris[,5])</pre>
```

unmap

Indicator Variables given Classification

Description

Converts a classification into a matrix of indicator variables.

Usage

```
unmap(classification, groups=NULL, noise=NULL, ...)
```

Arguments

classification	A numeric or character vector. Typically the distinct entries of this vector would represent a classification of observations in a data set.
groups	A numeric or character vector indicating the groups from which classification is drawn. If not supplied, the default is to assumed to be the unique entries of classification.
noise	A single numeric or character value used to indicate the value of groups corresponding to noise.
	Catches unused arguments in indirect or list calls via do.call.

Value

An n by m matrix of (0,1) indicator variables, where n is the length of classification and m is the number of unique values or symbols in classification. Columns are labeled by the unique values in classification, and the [i,j]th entry is l if classification[i] is the jth unique value or symbol in sorted order classification. If a noise value of symbol is designated, the corresponding indicator variables are relocated to the last column of the matrix.

- C. Fraley and A. E. Raftery (2002). Model-based clustering, discriminant analysis, and density estimation. *Journal of the American Statistical Association 97:611-631*.
- C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

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See Also

```
map, estep, me
```

Examples

```
z <- unmap(iris[,5])
z[1:5, ]
emEst <- me(modelName = "VVV", data = iris[,-5], z = z)
emEst$z[1:5,]
map(emEst$z)</pre>
```

wreath

Data Simulated from a 14-Component Mixture

Description

A dataset consisting of 1000 observations drawn from a 14-component normal mixture in which the covariances of the components have the same size and shape but differ in orientation.

Usage

```
data(wreath)
```

- C. Fraley, A. E. Raftery and R. Wehrens (2005). Incermental model-based clustering for large datasets with small clusters. *Journal of Computational and Graphical Statistics* 14:1:18.
- C. Fraley, A. E. Raftery, T. B. Murphy and L. Scrucca (2012). mclust Version 4 for R: Normal Mixture Modeling for Model-Based Clustering, Classification, and Density Estimation. Technical Report No. 597, Department of Statistics, University of Washington.

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