Package 'mclust'

April 29, 2024

Version 6.1.1 **Date** 2024-04-29

```
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, classification, 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 (>= 1.4), rmarkdown (>= 2.10), mix (>= 1.0), geometry
      (>= 0.4), MASS
License GPL (>= 2)
URL https://mclust-org.github.io/mclust/
VignetteBuilder knitr
Repository CRAN
ByteCompile true
NeedsCompilation yes
LazyData yes
Encoding UTF-8
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Date/Publication 2024-04-29 16:40:02 UTC
```

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Description

Gaussian finite mixture models estimated 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. See also:

- Mclust for clustering;
- MclustDA for supervised classification;
- MclustSSC for semi-supervised classification;
- densityMclust for density estimation.

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Author(s)

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References

Scrucca L., Fraley C., Murphy T. B. and Raftery A. E. (2023) *Model-Based Clustering, Classification, and Density Estimation Using mclust in R*. Chapman & Hall/CRC, ISBN: 978-1032234953, https://mclust-org.github.io/book/

Scrucca L., Fop M., Murphy T. B. and Raftery A. E. (2016) mclust 5: clustering, classification and density estimation using Gaussian finite mixture models, *The R Journal*, 8/1, pp. 289-317.

Fraley C. and Raftery A. E. (2002) Model-based clustering, discriminant analysis and density estimation, *Journal of the American Statistical Association*, 97/458, pp. 611-631.

Examples

```
# 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)</pre>
```

acidity

Acidity data

Description

Acidity index measured in a sample of 155 lakes in the Northeastern United States. Following Crawford et al. (1992, 1994), the data are expressed as log(ANC+50), where ANC is the acidity neutralising capacity value. 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)
```

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Source

https://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.

adjustedRandIndex

Adjusted Rand Index

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.

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, pp. 193-218.

See Also

classError, mapClass, table

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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])</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)
```

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.

Test 1D 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.

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Examples

```
data(Baudry_etal_2010_JCGS_examples)

output <- clustCombi(data = 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)</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, ...)
```

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.

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See Also

mclustBIC, nVarParams, mclustModelNames.

Examples

```
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)
# do.call("bic", emEst) ## alternative call</pre>
```

BrierScore

Brier score to assess the accuracy of probabilistic predictions

Description

The Brier score is a proper score function that measures the accuracy of probabilistic predictions.

Usage

```
BrierScore(z, class)
```

Arguments

Z

a matrix containing the predicted probabilities of each observation to be classified in one of the classes. Thus, the number of rows must match the length of class, and the number of columns the number of known classes.

class

a numeric, character vector or factor containing the known class labels for each observation. If class is a factor, the number of classes is nlevels(class) with classes levels(class). If class is a numeric or character vector, the number of classes is equal to the number of classes obtained via unique(class).

Details

The Brier Score is the mean square difference between the true classes and the predicted probabilities.

This function implements the original multi-class definition by Brier (1950), normalized to [0, 1] as in Kruppa et al (2014). The formula is the following:

$$BS = \frac{1}{2n} \sum_{i=1}^{n} \sum_{k=1}^{K} (C_{ik} - p_{ik})^{2}$$

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where n is the number of observations, K the number of classes, $C_{ik} = \{0, 1\}$ the indicator of class k for observation i, and p_{ik} is the predicted probability of observation i to belong to class k.

The above formulation is applicable to multi-class predictions, including the binary case. A small value of the Brier Score indicates high prediction accuracy.

The Brier Score is a strictly proper score (Gneiting and Raftery, 2007), which means that it takes its minimal value only when the predicted probabilities match the empirical probabilities.

References

Brier, G.W. (1950) Verification of forecasts expressed in terms of probability. *Monthly Weather Review*, 78 (1): 1-3.

Gneiting, G. and Raftery, A. E. (2007) Strictly proper scoring rules, prediction, and estimation. *Journal of the American Statistical Association* 102 (477): 359-378.

Kruppa, J., Liu, Y., Diener, H.-C., Holste, T., Weimar, C., Koonig, I. R., and Ziegler, A. (2014) Probability estimation with machine learning methods for dichotomous and multicategory outcome: Applications. *Biometrical Journal*, 56 (4): 564-583.

See Also

cvMclustDA

```
# multi-class case
class \leftarrow factor(c(5,5,5,2,5,3,1,2,1,1), levels = 1:5)
probs <- matrix(c(0.15, 0.01, 0.08, 0.23, 0.01, 0.23, 0.59, 0.02, 0.38, 0.45,
                  0.36, 0.05, 0.30, 0.46, 0.15, 0.13, 0.06, 0.19, 0.27, 0.17,
                  0.40, 0.34, 0.18, 0.04, 0.47, 0.34, 0.32, 0.01, 0.03, 0.11,
                  0.04, 0.04, 0.09, 0.05, 0.28, 0.27, 0.02, 0.03, 0.12, 0.25,
                  0.05, 0.56, 0.35, 0.22, 0.09, 0.03, 0.01, 0.75, 0.20, 0.02),
                nrow = 10, ncol = 5)
cbind(class, probs, map = map(probs))
BrierScore(probs, class)
# two-class case
class \leftarrow factor(c(1,1,1,2,2,1,1,2,1,1), levels = 1:2)
probs <- matrix(c(0.91, 0.4, 0.56, 0.27, 0.37, 0.7, 0.97, 0.22, 0.68, 0.43,
                  0.09, 0.6, 0.44, 0.73, 0.63, 0.3, 0.03, 0.78, 0.32, 0.57),
                nrow = 10, ncol = 2)
cbind(class, probs, map = map(probs))
BrierScore(probs, class)
# two-class case when predicted probabilities are constrained to be equal to
# 0 or 1, then the (normalized) Brier Score is equal to the classification
# error rate
probs <- ifelse(probs > 0.5, 1, 0)
cbind(class, probs, map = map(probs))
BrierScore(probs, class)
classError(map(probs), class)$errorRate
```

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```
# plot Brier score for predicted probabilities in range [0,1]
class <- factor(rep(1, each = 100), levels = 0:1)</pre>
prob <- seq(0, 1, by = 0.01)
brier <- sapply(prob, function(p)</pre>
  { z \leftarrow matrix(c(1-p,p), nrow = length(class), ncol = 2, byrow = TRUE)}
    BrierScore(z, class)
plot(prob, brier, type = "1", main = "Scoring all one class",
     xlab = "Predicted probability", ylab = "Brier score")
# brier score for predicting balanced data with constant prob
class <- factor(rep(c(1,0), each = 50), levels = 0:1)
prob <- seq(0, 1, by = 0.01)
brier <- sapply(prob, function(p)</pre>
  { z \leftarrow matrix(c(1-p,p), nrow = length(class), ncol = 2, byrow = TRUE)}
    BrierScore(z, class)
  })
plot(prob, brier, type = "l", main = "Scoring balanced classes",
     xlab = "Predicted probability", ylab = "Brier score")
# brier score for predicting unbalanced data with constant prob
class <- factor(rep(c(0,1), times = c(90,10)), levels = 0:1)
prob <- seq(0, 1, by = 0.01)
brier <- sapply(prob, function(p)</pre>
  { z \leftarrow matrix(c(1-p,p), nrow = length(class), ncol = 2, byrow = TRUE)}
    BrierScore(z, class)
plot(prob, brier, type = "1", main = "Scoring unbalanced classes",
     xlab = "Predicted probability", ylab = "Brier score")
```

cdens

Component Density for Parameterized MVN Mixture Models

Description

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

Usage

```
cdens(data, modelName, parameters, logarithm = FALSE, 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.

modelName

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

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

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.

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

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|
```

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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, ...)
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, ...)
cdensXXI(data, logarithm = FALSE, parameters, warn = NULL, ...)
cdensXXX(data, logarithm = FALSE, 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.

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.

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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 computations 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.

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.

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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.

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 bisection linear search algorithm.

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.

Author(s)

Luca Scrucca

See Also

densityMclust, plot.densityMclust.

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

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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

Computes the errore rate of a given classification relative to the known classes, and the location of misclassified data points.

Usage

```
classError(classification, class)
```

Arguments

classification A numeric, character vector or factor specifying the predicted class labels. Must

have the same length as class.

class A numeric, character vector or factor of known true class labels. Must have the

same length as classification.

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Details

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

Value

A list with the following two components:

misclassified The indexes of the misclassified data points in a minimum error mapping be-

tween the predicted classification and the known true classes.

errorRate The error rate corresponding to a minimum error mapping between the predicted

classification and the known true classes.

See Also

```
map mapClass, table
```

Examples

classPriorProbs

Estimation of class prior probabilities by EM algorithm

Description

A simple procedure to improve the estimation of class prior probabilities when the training data does not reflect the true a priori probabilities of the target classes. The EM algorithm used is described in Saerens et al (2002).

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Usage

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 used.

itmax an integer value specifying the maximal number of EM iterations.

eps a scalar specifying the tolerance associated with deciding when to terminate the

EM iterations.

Details

The estimation procedure employes an EM algorithm as described in Saerens et al (2002).

Value

A vector of class prior estimates which can then be used in the predict.MclustDA to improve predictions.

References

Saerens, M., Latinne, P. and Decaestecker, C. (2002) Adjusting the outputs of a classifier to new a priori probabilities: a simple procedure, *Neural computation*, 14 (1), 21–41.

See Also

MclustDA, predict.MclustDA

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```
class_train <- factor(sample(0:1, size = n_{train}, prob = c(0.5, 0.5), replace = TRUE))
x_train <- ifelse(class_train == 1, rnorm(n_train, mean = 3, sd = 1),</pre>
                                     rnorm(n_train, mean = 0, sd = 1))
hist(x_train[class_train==0], breaks = 11, xlim = range(x_train),
     main = "", xlab = "x",
     col = adjustcolor("dodgerblue2", alpha.f = 0.5), border = "white")
hist(x_train[class_train==1], breaks = 11, add = TRUE,
     col = adjustcolor("red3", alpha.f = 0.5), border = "white")
box()
# fit a MclustDA model
mod <- MclustDA(x_train, class_train)</pre>
summary(mod, parameters = TRUE)
# test set performance
pred <- predict(mod, newdata = x)</pre>
classError(pred$classification, class)$error
BrierScore(pred$z, class)
# compute performance over a grid of prior probs
priorProp <- seq(0.01, 0.99, by = 0.01)
CE <- BS <- rep(as.double(NA), length(priorProp))</pre>
for(i in seq(priorProp))
  pred <- predict(mod, newdata = x, prop = c(1-priorProp[i], priorProp[i]))</pre>
  CE[i] <- classError(pred$classification, class = class)$error</pre>
  BS[i] <- BrierScore(pred$z, class)</pre>
}
# estimate the optimal class prior probs
(priorProbs <- classPriorProbs(mod, x))</pre>
pred <- predict(mod, newdata = x, prop = priorProbs)</pre>
# compute performance at the estimated class prior probs
classError(pred$classification, class = class)$error
BrierScore(pred$z, class)
matplot(priorProp, cbind(CE,BS), type = "1", lty = 1, lwd = 2,
        xlab = "Class prior probability", ylab = "", ylim = c(0, max(CE, BS)),
        panel.first =
          { abline(h = seq(0,1,by=0.05), col = "grey", lty = 3)}
            abline(v = seq(0,1,by=0.05), col = "grey", lty = 3)
          })
abline(v = mod$prop[2], lty = 2)
                                               # training prop
abline(v = mean(class==1), lty = 4)
                                               # test prop (usually unknown)
abline(v = priorProbs[2], lty = 3, lwd = 2)
                                                  # estimated prior probs
legend("topleft", legend = c("ClassError", "BrierScore"),
       col = 1:2, lty = 1, lwd = 2, inset = 0.02)
# Summary of results:
priorProp[which.min(CE)] # best prior of class 1 according to classification error
priorProp[which.min(BS)] # best prior of class 1 according to Brier score
priorProbs
                         # optimal estimated class prior probabilities
```

clPairs 21

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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

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").
cex	A vector of numerical values specifying the size of the plotting symbol for each unique class in classification. Values in cex correspond to classes in order of appearance in the sequence of observations (the order used by the function unique). By default cex = 1 for all classes is used.
labels	A vector of character strings for labelling the variables. The default is to use the column dimension names of data.
cex.labels	A numerical value specifying the size of the text labels.
gap	An argument specifying the distance between subplots (see pairs).
grid	A logical specifying if grid lines should be added to panels (see grid).
х,у	The x and y co-ordinates with respect to a graphic device having plotting region coordinates $par("usr" = c(0,1,0,1))$.

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class	The class labels.
box	A logical, if TRUE then a box is drawn around the current plot figure.
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.

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.

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.

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(object = NULL, data = NULL, ...)
```

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Arguments

object An object returned by Mclust giving the optimal (according to BIC) parame-

ters, conditional probabilities, and log-likelihood, together with the associated classification and its uncertainty. If not provided, the data argument must be

specified.

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. If the object argument is not provided, the

function Mclust is applied to the given data to fit a mixture model.

... Optional arguments to be passed to called functions. Notably, any argument

(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, etc.) to be passed to Mclust in case object = 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.

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.

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See Also

```
plot.clustCombi
```

```
data(Baudry_etal_2010_JCGS_examples)
# run Mclust using provided data
output <- clustCombi(data = ex4.1)</pre>
# or run Mclust and then clustcombi on the returned object
mod <- Mclust(ex4.1)</pre>
output <- clustCombi(mod)</pre>
output
summary(output)
# run Mclust using provided data and any further optional argument provided
output <- clustCombi(data = ex4.1, modelName = "EEV", G = 1:15)</pre>
# plot the hierarchy of combined solutions
plot(output, what = "classification")
# plot some "entropy plots" which may help one to select the number of classes
plot(output, what = "entropy")
# plot the tree structure obtained from combining mixture components
plot(output, what = "tree")
# the selected model and number of components obtained from Mclust using BIC
output$MclustOutput
# the matrix whose [i,k]th entry is the probability that i-th observation in
# the data belongs to the k-th class according to the BIC solution
head( output$combiz[[output$MclustOutput$G]] )
# the matrix whose [i,k]th entry is the probability that i-th observation in
# the data belongs to the k-th class according to the first combined 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
```

clustCombiOptim 25

head(<pre>output\$classification[[5]]</pre>)
-------	--	---

clustCombiOptim	Optimal number of clusters obtained by combining mixture compo-
	nents

Description

Return the optimal number of clusters by combining mixture components based on the entropy method discussed in the reference given below.

Usage

```
clustCombiOptim(object, reg = 2, plot = FALSE, ...)
```

Arguments

object	An object of class 'clustCombi' resulting from a call to clustCombi.
reg	The number of parts of the piecewise linear regression for the entropy plots. Choose 2 for a two-segment piecewise linear regression model (i.e. 1 changepoint), and 3 for a three-segment piecewise linear regression model (i.e. 3 change-points).
plot	Logical, if TRUE an entropy plot is also produced.
	Further arguments passed to or from other methods.

Value

The function returns a list with the following components:

```
numClusters.combi
```

The estimated number of clusters.

z.combi A matrix whose [i,k]th entry is the probability that observation i in the data

belongs to the *k*th cluster.

cluster.combi The clustering labels.

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
```

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Examples

```
data(Baudry_etal_2010_JCGS_examples)
output <- clustCombi(data = ex4.1)
combiOptim <- clustCombiOptim(output)
str(combiOptim)

# plot optimal clustering with alpha color transparency proportional to uncertainty
zmax <- apply(combiOptim$z.combi, 1, max)
col <- mclust.options("classPlotColors")[combiOptim$cluster.combi]
vadjustcolor <- Vectorize(adjustcolor)
alphacol = (zmax - 1/combiOptim$numClusters.combi)/(1-1/combiOptim$numClusters.combi)
col <- vadjustcolor(col, alpha.f = alphacol)
plot(ex4.1, col = col, pch = mclust.options("classPlotSymbols")[combiOptim$cluster.combi])</pre>
```

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.

Author(s)

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

combiTree 27

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$G # Mclust/BIC selected 6 classes
par(mfrow=c(2,2))
combiM0 <- diag(6) # is the identity matrix</pre>
# no merging: plot the initial solution, given by z
combiPlot(ex4.1, MclustOutput$z, combiM0, cex = 3)
title("No combining")
combiM1 <- combMat(6, 1, 2) # let's merge classes labeled 1 and 2</pre>
combiM1
combiPlot(ex4.1, MclustOutput$z, combiM1)
title("Combine 1 and 2")
# let's merge classes labeled 1 and 2, and then components labeled (in this
# new 5-classes combined solution) 1 and 2
combiM2 <- combMat(5, 1, 2) %*% combMat(6, 1, 2)</pre>
combiM2
combiPlot(ex4.1, MclustOutput$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:")
```

combiTree

Tree structure obtained from combining mixture components

Description

The method implemented in clustCombi can be used for combining Gaussian mixture components for clustering. This provides a hierarchical structure which can be graphically represented as a tree.

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Usage

Arguments

object	An object of class 'clustCombi' resulting from a call to clustCombi.
type	A string specifying the dendrogram's type. Possible values are "triangle" (default), and "rectangle".
yaxis	A string specifying the quantity used to draw the vertical axis. Possible values are "entropy" (default), and "step".
edgePar	A list of plotting parameters. See dendrogram.
	Further arguments passed to or from other methods.

Value

The function always draw a tree and invisibly returns an object of class 'dendrogram' for fine tuning.

Author(s)

L. Scrucca

See Also

clustCombi

```
data(Baudry_etal_2010_JCGS_examples)
output <- clustCombi(data = ex4.1)
combiTree(output)
combiTree(output, type = "rectangle")
combiTree(output, yaxis = "step")
combiTree(output, type = "rectangle", yaxis = "step")</pre>
```

combMat 29

ng Matrix

Description

Create a combining matrix

Usage

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

Arguments

К	The original number of classes: the matrix will define a combining from K to (K-1) classes.
11	Label of one of the two classes to be combined.
12	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
```

See Also

clustCombi, combiPlot

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

Description

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

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Usage

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

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.

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 parameters

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.

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.

A numeric vector of values in (0,1) giving the uncertainty of each data point. If uncertainty

present argument z will be ignored.

what Choose from one of the following three options: "classification" (default),

"error", "uncertainty".

A logical indicating whether or not to add ellipses with axes corresponding to addEllipses

the within-cluster covariances in case of "classification" or "uncertainty"

plots.

fillEllipses A logical specifying whether or not to fill ellipses with transparent colors when

addEllipses = TRUE.

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").

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covw 31

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	A numerical value 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.

Value

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.

See Also

```
clPairs, randProj, mclust2Dplot, mclust.options
```

Examples

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

32 crimcoords

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.

normalize 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

Examples

```
# 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))</pre>
```

crimcoords

Discriminant coordinates data projection

Description

Compute the discriminant coordinates or crimcoords obtained by projecting the observed data from multiple groups onto the discriminant subspace. The optimal projection subspace is given by the linear transformation of the original variables that maximizes the ratio of the between-groups covariance (which represents groups separation) to the pooled within-group covariance (which represents within-group dispersion).

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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.

classification A vector (numerical, character string, or factor) giving the groups classification

(either the known class labels or the estimated clusters) for the observed data.

numdir An integer value specifying the number of directions of the discriminant sub-

space to return. If not provided, the maximal number of directions are returned (which is given by the number of non-null eigenvalues, the minimum among the number of variables and the number of groups minus one). However, since the effectiveness of the discriminant coordinates in highlighting the separation of groups is decreasing, it might be useful to provide a smaller value, say 2 or 3.

unbiased A logical specifying if unbiased estimates should be used for the between-

groups and within-groups covariances. By default unbiased = FALSE so MLE estimates are used. Note that the use of unbiased or MLE estimates only changes the eigenvalues and eigenvectors of the generalized eigendecomposition by a constant of proportionality, so the discriminant coordinates or crimcoords are

essentially the same.

object, x An object of class crimcoords as returned by crimcoords() function.

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

Value

A list of class crimcoords with the following components:

means A matrix of within-groups means.

B The between-groups covariance matrix.

W The pooled within-groups covariance matrix.

evalues A vector of eigenvalues.

basis A matrix of eigenvectors specifying the basis of the discriminant subspace.

projection A matrix of projected data points onto the discriminant subspace.

classification A vector giving the groups classification.

34 cross

Author(s)

Luca Scrucca < luca.scrucca@unipg.it>

References

Gnanadesikan, R. (1977) *Methods for Statistical Data Analysis of Multivariate Observations*. John Wiley 1& Sons, Sec. 4.2.

Flury, B. (1997) A First Course in Multivariate Statistics. Springer, Sec. 7.3.

See Also

MclustDR, clPairs.

Examples

```
# discriminant coordinates for the iris data using known classes
data("iris")
CRIMCOORDS = crimcoords(iris[,-5], iris$Species)
summary(CRIMCOORDS)
plot(CRIMCOORDS)
# banknote data
data("banknote")
# discriminant coordinate on known classes
CRIMCOORDS = crimcoords(banknote[,-1], banknote$Status)
summary(CRIMCOORDS)
plot(CRIMCOORDS)
# discriminant coordinates on estimated clusters
mod = Mclust(banknote[,-1])
CRIMCOORDS = crimcoords(banknote[,-1], mod$classification)
summary(CRIMCOORDS)
plot(CRIMCOORDS)
plot(CRIMCOORDS$projection, type = "n")
text(CRIMCOORDS$projection, cex = 0.8,
     labels = strtrim(banknote$Status, 2),
     col = mclust.options("classPlotColors")[1:mod$G][mod$classification])
```

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)
```

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Examples

cvMclustDA

MclustDA cross-validation

Description

V-fold cross-validation for classification models based on Gaussian finite mixture modelling.

Usage

Arguments

object	An object of class 'MclustDA' resulting from a call to MclustDA.
nfold	An integer specifying the number of folds (by defaul 10-fold CV is used).
prop	A vector of class prior probabilities, which if not provided default to the class proportions in the training data.
verbose	A logical controlling if a text progress bar is displayed during the cross-validation procedure. By default is TRUE if the session is interactive, and FALSE otherwise.
	Further arguments passed to or from other methods.

Details

The function implements V-fold cross-validation for classification models fitted by MclustDA. Classification error and Brier score are the metrics returned, but other metrics can be computed using the output returned by this function (see Examples section below).

Value

The function returns a list with the following components:

classification a factor of cross-validated class labels.

z a matrix containing the cross-validated probabilities for class assignment.

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ce the cross-validation classification error.

se.ce the standard error of the cross-validated classification error.

brier the cross-validation Brier score.

se.brier the standard error of the cross-validated Brier score.

Author(s)

Luca Scrucca

See Also

MclustDA, predict.MclustDA, classError, BrierScore

```
# Iris data
Class <- iris$Species
X <- iris[,1:4]
## EDDA model with common covariance (essentially equivalent to linear discriminant analysis)
irisEDDA <- MclustDA(X, Class, modelType = "EDDA", modelNames = "EEE")</pre>
cv <- cvMclustDA(irisEDDA)</pre>
                                                        # 10-fold CV (default)
str(cv)
cv <- cvMclustDA(irisEDDA, nfold = length(Class)) # LOO-CV</pre>
str(cv)
## MclustDA model selected by BIC
irisMclustDA <- MclustDA(X, Class)</pre>
                                                        # 10-fold CV (default)
cv <- cvMclustDA(irisMclustDA)</pre>
str(cv)
# Banknote data
data("banknote")
Class <- banknote$Status</pre>
X <- banknote[,2:7]</pre>
## EDDA model selected by BIC
banknoteEDDA <- MclustDA(X, Class, modelType = "EDDA")</pre>
cv <- cvMclustDA(banknoteEDDA)</pre>
                                                        # 10-fold CV (default)
str(cv)
(ConfusionMatrix <- table(Pred = cv$classification, Class))</pre>
TP <- ConfusionMatrix[1,1]</pre>
FP <- ConfusionMatrix[1,2]</pre>
FN <- ConfusionMatrix[2,1]</pre>
TN <- ConfusionMatrix[2,2]
(Sensitivity <- TP/(TP+FN))
(Specificity <- TN/(FP+TN))
```

decomp2sigma 37

decomp2sigma	Convert mixture component covariances to matrix form
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

guments	
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 kth component in an MVN mixture model.

See Also

```
sigma2decomp
```

```
meEst <- meVEV(iris[,-5], unmap(iris[,5]))
names(meEst)
meEst$parameters$variance

dec <- meEst$parameters$variance</pre>
```

38 defaultPrior

defaultPrior

Default conjugate prior for Gaussian mixtures

Description

Default conjugate prior specification for Gaussian mixtures.

Usage

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

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 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

"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.

... 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.

defaultPrior 39

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.

See Also

mclustBIC, me, mstep, priorControl

40 dens

dens	Density for Parameterized MVN Mixtures	

Description

Computes densities of observations in parameterized MVN mixtures.

Usage

```
dens(data, modelName, parameters, logarithm = FALSE, 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.
modelName	A character string indicating the model. The help file for ${\tt mclustModelNames}$ describes the available models.
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 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.
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.
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 vector whose *i*th component is the density of the *ith* observation in data in the MVN mixture specified by parameters.

See Also

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

densityMclust 41

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, ..., plot = TRUE)
```

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.
plot	A logical value specifying if the estimated density should be plotted. For more contols on the resulting graph see the associated plot.densityMclust method.

Value

An object of class densityMclust, which inherits from Mclust. This contains all the components described in Mclust and the additional element:

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

Author(s)

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

References

Scrucca L., Fraley C., Murphy T. B. and Raftery A. E. (2023) *Model-Based Clustering, Classification, and Density Estimation Using mclust in R.* Chapman & Hall/CRC, ISBN: 978-1032234953, https://mclust-org.github.io/book/

Scrucca L., Fop M., Murphy T. B. and Raftery A. E. (2016) mclust 5: clustering, classification and density estimation using Gaussian finite mixture models, *The R Journal*, 8/1, pp. 289-317.

Fraley C. and Raftery A. E. (2002) Model-based clustering, discriminant analysis and density estimation, *Journal of the American Statistical Association*, 97/458, pp. 611-631.

See Also

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

Examples

```
dens <- densityMclust(faithful$waiting)</pre>
summary(dens)
summary(dens, parameters = TRUE)
plot(dens, what = "BIC", legendArgs = list(x = "topright"))
plot(dens, what = "density", data = faithful$waiting)
dens <- densityMclust(faithful, modelNames = "EEE", G = 3, plot = FALSE)</pre>
summary(dens)
summary(dens, parameters = TRUE)
plot(dens, what = "density", data = faithful,
     drawlabels = FALSE, points.pch = 20)
plot(dens, what = "density", type = "hdr")
plot(dens, what = "density", type = "hdr", prob = c(0.1, 0.9))
plot(dens, what = "density", type = "hdr", data = faithful)
plot(dens, what = "density", type = "persp")
dens <- densityMclust(iris[,1:4], G = 2)</pre>
summary(dens, parameters = TRUE)
plot(dens, what = "density", data = iris[,1:4],
     col = "slategrey", drawlabels = FALSE, nlevels = 7)
plot(dens, what = "density", type = "hdr", data = iris[,1:4])
plot(dens, what = "density", type = "persp", col = grey(0.9))
```

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.
	Additional arguments.

Details

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

Author(s)

Luca Scrucca

References

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

Scrucca L., Fraley C., Murphy T. B. and Raftery A. E. (2023) *Model-Based Clustering, Classification, and Density Estimation Using mclust in R*. Chapman & Hall/CRC, ISBN: 978-1032234953, https://mclust-org.github.io/book/

See Also

densityMclust, plot.densityMclust.

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Examples

```
x <- faithful$waiting
dens <- densityMclust(x, plot = FALSE)
plot(dens, x, what = "diagnostic")
# or
densityMclust.diagnostic(dens, type = "cdf")
densityMclust.diagnostic(dens, type = "qq")</pre>
```

diabetes

Diabetes Data (flawed)

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.

Details

This dataset is *flawed* (compare with the reference) and it is provided here only for backward compatibility. A 5-variable version of the Reaven and Miller data is available in package **rrcov**. The *glucose* and *sspg* columns in this dataset are identical to the *fpg* and *insulin* columns, respectively in the **rrcov** version. The *insulin* column in this dataset differs from the *glucose* column in the **rrcov** version in one entry: observation 104 has the value 45 in the *insulin* column in this data, and 455 in the corresponding *glucose* column of the **rrcov** version.

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.

dmvnorm 45

dmvnorm Density of multivariate Gaussian distribution	
---	--

Description

Efficiently computes the density of observations for a generic multivariate Gaussian distribution.

Usage

```
dmvnorm(data, mean, sigma, log = 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.
mean	A vector of means for each variable.
sigma	A positive definite covariance matrix.
log	A logical value indicating whether or not the logarithm of the densities should be returned.

Value

A numeric vector whose *i*th element gives the density of the *ith* observation in data for the multivariate Gaussian distribution with parameters mean and sigma.

See Also

```
dnorm, dens
```

```
# univariate
ngrid <- 101
x <- seq(-5, 5, length = ngrid)
dens <- dmvnorm(x, mean = 1, sigma = 5)
plot(x, dens, type = "1")

# bivariate
ngrid <- 101
x1 <- x2 <- seq(-5, 5, length = ngrid)
mu <- c(1,0)
sigma <- matrix(c(1,0.5,0.5,2), 2, 2)
dens <- dmvnorm(as.matrix(expand.grid(x1, x2)), mu, sigma)
dens <- matrix(dens, ngrid, ngrid)
image(x1, x2, dens)
contour(x1, x2, dens, add = TRUE)</pre>
```

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dupPartition

Partition the data by grouping together duplicated data

Description

Duplicated data are grouped together to form a basic partition that can be used to start hierarchical agglomeration.

Usage

```
dupPartition(data)
```

Arguments

data

A numeric vector, matrix, or data frame of observations. If a matrix or data frame, rows correspond to observations (n) and columns correspond to variables (d).

Value

A vector of indices indicating the partition.

See Also

hc

Examples

```
dupPartition(iris[,1:4])
dupPartition(iris)
dupPartition(iris$Species)
```

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

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Arguments

modelName

parameters

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

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.

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

sumes no prior.

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 when com-

putations fail. The default is warn=FALSE.

... 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.

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

tion belonging to the *k*th 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.

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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.

See Also

```
emE, ..., emVVV, estep, me, mstep, mclust.options, do.call
```

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)
```

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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", "VEE", "EVE", "VVE", "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", "VEE", "EVE", "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.

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.

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.

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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, ...)
emVEE(data, parameters, prior = NULL, control = emControl(), warn = NULL, ...)
emEVE(data, parameters, prior = NULL, control = emControl(), warn = NULL, ...)
emVVE(data, parameters, prior = NULL, control = emControl(), warn = NULL, ...)
emEEV(data, parameters, prior = NULL, control = emControl(), warn = NULL, ...)
emVEV(data, parameters, prior = NULL, control = emControl(), warn = NULL, ...)
emEVV(data, parameters, prior = NULL, control = emControl(), warn = NULL, ...)
emVVV(data, parameters, prior = NULL, control = emControl(), warn = NULL, ...)
emXII(data, prior = NULL, 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 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. 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.

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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 *i*th observa-

tion 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.

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.

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
```

```
data(Baudry_etal_2010_JCGS_examples)
# run Mclust to get the MclustOutput
```

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```
output <- clustCombi(data = 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.</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)
errorBars(x, lower = n-se, upper = n+se, lwd = 2, col = "red3")</pre>
```

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```
# 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(data, modelName, 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.

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

describes the available models.

parameters 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.

tion 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.

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 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	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 computations.

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, ...)
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, ...)
```

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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.

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.

See Also

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

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

EuroUnemployment 57

EuroUnemployment

Unemployment data for European countries in 2014

Description

The data set contains unemployment rates for 31 European countries for the year 2014.

Usage

```
data(EuroUnemployment)
```

Format

A data frame with the following variables:

- **TUR** Total unemployment rate, i.e. percentage of unemployed persons aged 15-74 in the economically active population.
- **YUR** Youth unemployment rate, i.e. percentage of unemployed persons aged 15-24 in the economically active population.
- **LUR** Long-term unemployment rate, i.e. percentage of unemployed persons who have been unemployed for 12 months or more.

Source

Dataset downloaded from EUROSTAT https://ec.europa.eu/eurostat.

gmmhd

Identifying Connected Components in Gaussian Finite Mixture Models for Clustering

Description

Starting with the density estimate obtained from a fitted Gaussian finite mixture model, cluster cores are identified from the connected components at a given density level. Once cluster cores are identified, the remaining observations are allocated to those cluster cores for which the probability of cluster membership is the highest.

Usage

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Arguments

object An object returned by Mclust.

ngrid An integer specifying the number of grid points used to compute the density

levels.

dr A list of parameters used in the dimension reduction step.

classify A list of parameters used in the classification step.

x An object of class 'gmmhd' as returned by the function gmmhd.

what A string specifying the type of plot to be produced. See Examples section.

further arguments passed to or from other methods.

Details

Model-based clustering associates each component of a finite mixture distribution to a group or cluster. An underlying implicit assumption is that a one-to-one correspondence exists between mixture components and clusters. However, a single Gaussian density may not be sufficient, and two or more mixture components could be needed to reasonably approximate the distribution within a homogeneous group of observations.

This function implements the methodology proposed by Scrucca (2016) based on the identification of high density regions of the underlying density function. Starting with an estimated Gaussian finite mixture model, the corresponding density estimate is used to identify the cluster cores, i.e. those data points which form the core of the clusters. These cluster cores are obtained from the connected components at a given density level c. A mode function gives the number of connected components as the level c is varied. Once cluster cores are identified, the remaining observations are allocated to those cluster cores for which the probability of cluster membership is the highest.

The method usually improves the identification of non-Gaussian clusters compared to a fully parametric approach. Furthermore, it enables the identification of clusters which cannot be obtained by merging mixture components, and it can be straightforwardly extended to cases of higher dimensionality.

Value

A list of class gmmhd with the following components:

Mclust The input object of class "Mclust" representing an estimated Gaussian finite

mixture model.

MclustDA An object of class "MclustDA" containing the model used for the classification

step.

MclustDR An object of class "MclustDR" containing the dimension reduction step if per-

formed, otherwise NULL.

x The data used in the algorithm. This can be the input data or a projection if a

preliminary dimension reduction step is performed.

density The density estimated from the input Gaussian finite mixture model evaluated at

the input data.

con A list of connected components at each step.

gmmhd 59

nc	A vector giving the number of connected components (i.e. modes) at each step.
pn	Vector of values over a uniform grid of proportions of length ngrid.
qn	Vector of density quantiles corresponding to proportions pn.
рс	Vector of empirical proportions corresponding to quantiles qn.
clusterCores	Vector of cluster cores numerical labels; NAs indicate that an observation does not belong to any cluster core.
clusterCores	Vector of numerical labels giving the final clustering.
numClusters	An integer giving the number of clusters.

Author(s)

Luca Scrucca < luca.scrucca@unipg.it>

References

Scrucca, L. (2016) Identifying connected components in Gaussian finite mixture models for clustering. *Computational Statistics & Data Analysis*, 93, 5-17.

See Also

Mclust

```
data(faithful)
mod <- Mclust(faithful)
summary(mod)
plot(as.densityMclust(mod), faithful, what = "density",
        points.pch = mclust.options("classPlotSymbols")[mod$classification],
        points.col = mclust.options("classPlotColors")[mod$classification])

GMMHD <- gmmhd(mod)
summary(GMMHD)

plot(GMMHD, what = "mode")
plot(GMMHD, what = "cores")
plot(GMMHD, what = "clusters")</pre>
```

60 GvHD

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.

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.

hc 61

Examples

```
data(GvHD)
dat <- GvHD.pos[1:500,] # only a few lines for a quick example
output <- clustCombi(data = dat)
output # is of class clustCombi
# plot the hierarchy of combined solutions
plot(output, what = "classification")
# plot some "entropy plots" which may help one to select the number of classes
plot(output, what = "entropy")
# plot the tree structure obtained from combining mixture components
plot(output, what = "tree")</pre>
```

hc

Model-based Agglomerative Hierarchical Clustering

Description

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

Usage

```
hc(data,
    modelName = "VVV",
    use = "VARS",
    partition = dupPartition(data),
    minclus = 1, ...)
## S3 method for class 'hc'
as.hclust(x, ...)
```

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 (n) and columns correspond to variables (d).

modelName

A character string indicating the model to be used in model-based agglomerative hierarchical clustering.

Possible models are:

"E" equal variance (one-dimensional);

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

"EII" spherical, equal volume;

"VII" spherical, unequal volume;

62 hc

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

"VVV" ellipsoidal, varying volume, shape, and orientation (default).

If hc() is used for initialization of EM algorithm then the default is taken from mclust.options("hcModelName"). See mclust.options.

use

A character string specifying the type of input variables/data transformation to be used for model-based agglomerative hierarchical clustering.

Possible values are:

"VARS" original variables (default);

"STD" standardized variables (centered and scaled);

"SPH" sphered variables (centered, scaled and 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.

If hc() is used for initialization of EM algorithm then the default is taken from mclust.options("hcUse"). See mclust.options.

For further details see Scrucca and Raftery (2015).

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. Starting with version 5.4.8, by default the function dupPartition is used to start with all duplicated observations in the same group, thereby keeping duplicates in the same group throughout the modelling process.

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.

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

An object of class 'hc' resulting from a call to hc().

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

The function hc() returns 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. Several other informations are also returned as attributes.

The method as.hclust.hc() can be used to convert the input object from class 'hc' to class 'hclust'.

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Note

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

References

Banfield J. D. and Raftery A. E. (1993). Model-based Gaussian and non-Gaussian Clustering. *Biometrics*, 49:803-821.

Fraley C. (1998). Algorithms for model-based Gaussian hierarchical clustering. *SIAM Journal on Scientific Computing*, 20:270-281.

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

Scrucca L. and Raftery A. E. (2015). Improved initialisation of model-based clustering using Gaussian hierarchical partitions. *Advances in Data Analysis and Classification*, 9/4:447-460.

See Also

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

Examples

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

clPairs(iris[,-5], classification = cl[,"2"])
clPairs(iris[,-5], classification = cl[,"3"])</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 = NULL, minclus=1, ...)
hcV(data, partition = NULL, minclus = 1, alpha = 1, ...)
hcEII(data, partition = NULL, minclus = 1, ...)
hcVII(data, partition = NULL, minclus = 1, alpha = 1, ...)
hcEEE(data, partition = NULL, minclus = 1, ...)
hcVVV(data, partition = NULL, minclus = 1, alpha = 1, beta = 1, ...)
```

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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.
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*.

See Also

hc, hclass hcRandomPairs

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

par(pty = "s", mfrow = c(1,1))
clPairs(iris[,-5],cl=cl[,"2"])
clPairs(iris[,-5],cl=cl[,"3"])</pre>
```

hclass 65

```
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)</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 classifications 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.

See Also

```
hc, hcE
```

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

par(pty = "s", mfrow = c(1,1))
clPairs(iris[,-5],cl=cl[,"2"])
clPairs(iris[,-5],cl=cl[,"3"])</pre>
```

66 hcRandomPairs

hcRandomPairs	Random hierarchical structure

Description

Create a hierarchical structure using a random hierarchical partition of the data.

Usage

```
hcRandomPairs(data, seed = NULL, ...)
```

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.

See Also

```
hc, hclass hcVVV
```

```
data <- iris[,1:4]
randPairs <- hcRandomPairs(data)
str(randPairs)
# start model-based clustering from a random partition
mod <- Mclust(data, initialization = list(hcPairs = randPairs))
summary(mod)</pre>
```

hdrlevels 67

hdrlevels

Highest Density Region (HDR) Levels

Description

Compute the levels of Highest Density Regions (HDRs) for any density and probability levels.

Usage

hdrlevels(density, prob)

Arguments

density A vector of density values computed on a set of (observed) evaluation points.

prob A vector of probability levels in the range [0, 1].

Details

From Hyndman (1996), let f(x) be the density function of a random variable X. Then the $100(1-\alpha)\%$ HDR is the subset $R(f_{\alpha})$ of the sample space of X such that

$$R(f_{\alpha}) = x : f(x) \ge f_{\alpha}$$

where f_α is the largest constant such that $Pr(X \in R(f_\alpha)) \geq 1 - \alpha$

Value

The function returns a vector of density values corresponding to HDRs at given probability levels.

Author(s)

L. Scrucca

References

Rob J. Hyndman (1996) Computing and Graphing Highest Density Regions. *The American Statistician*, 50(2):120-126.

See Also

plot.densityMclust

68 hdrlevels

```
# Example: univariate Gaussian
x <- rnorm(1000)
f <- dnorm(x)</pre>
a \leftarrow c(0.5, 0.25, 0.1)
(f_a \leftarrow hdrlevels(f, prob = 1-a))
plot(x, f)
abline(h = f_a, lty = 2)
text(max(x), f_a, labels = paste0("f_", a), pos = 3)
mean(f > f_a[1])
range(x[which(f > f_a[1])])
qnorm(1-a[1]/2)
mean(f > f_a[2])
range(x[which(f > f_a[2])])
qnorm(1-a[2]/2)
mean(f > f_a[3])
range(x[which(f > f_a[3])])
qnorm(1-a[3]/2)
# Example 2: univariate Gaussian mixture
set.seed(1)
cl <- sample(1:2, size = 1000, prob = c(0.7, 0.3), replace = TRUE)
x \leftarrow ifelse(cl == 1,
            rnorm(1000, mean = 0, sd = 1),
            rnorm(1000, mean = 4, sd = 1))
f <- 0.7*dnorm(x, mean = 0, sd = 1) + 0.3*dnorm(x, mean = 4, sd = 1)
a <- 0.25
(f_a \leftarrow hdrlevels(f, prob = 1-a))
plot(x, f)
abline(h = f_a, lty = 2)
text(max(x), f_a, labels = paste0("f_", a), pos = 3)
mean(f > f_a)
# find the regions of HDR
ord <- order(x)</pre>
f <- f[ord]
x \leftarrow x[ord]
x_a <- x[f > f_a]
j <- which.max(diff(x_a))</pre>
region1 <- x_a[c(1,j)]
region2 <- x_a[c(j+1, length(x_a))]
plot(x, f, type = "l")
abline(h = f_a, lty = 2)
abline(v = region1, lty = 3, col = 2)
abline(v = region2, lty = 3, col = 3)
```

hypvol 69

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	v	v	v	v	_

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 de-

sired rather than the hypervolume itself. The default is to return the hypervol-

ume.

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*.

See Also

mclustBIC

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

70 icl

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.

See Also

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

```
mod <- Mclust(iris[,1:4])
icl(mod)</pre>
```

imputeData 71

imputeData	Missing data imputation via the mix package	

Description

Imputes missing data using the mix package.

Usage

```
imputeData(data, categorical = NULL, seed = NULL, verbose = interactive())
```

Arguments

O	
data	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 data 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 number generator in mix . By default, a seed is chosen uniformly in the interval (.Machine\$integer.max/1024, .Machine\$integer.max).
verbose	A logical, if TRUE reports info about iterations of the algorithm.

Value

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

References

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

See Also

```
impute Pairs\\
```

```
# Note that package 'mix' must be installed
data(stlouis, package = "mix")

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

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

72 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

Arguments

data	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.
dataImp	The dataset data 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.

logLik.Mclust 73

Value

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

References

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

See Also

```
pairs, imputeData
```

Examples

```
# Note that package 'mix' must be installed
data(stlouis, package = "mix")

# 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").

74 logLik.MclustDA

Author(s)

Luca Scrucca

See Also

Mclust.

Examples

```
irisMclust <- Mclust(iris[,1:4])
summary(irisMclust)
logLik(irisMclust)</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").

Author(s)

Luca Scrucca

See Also

MclustDA.

logsumexp 75

Examples

```
irisMclustDA <- MclustDA(iris[,1:4], iris$Species)
summary(irisMclustDA)
logLik(irisMclustDA)</pre>
```

logsumexp

Log sum of exponentials

Description

Efficient implementation (via Fortran) of the log-sum-exp function.

Usage

logsumexp(x, v = NULL)

Arguments

x a matrix of dimension $n \times k$ of numerical values. If a vector is provided, it is converted to a single-row matrix.

an optional vector of length k of numerical values to be added to each row of x matrix. If not provided, a vector of zeros is used.

Details

Given the matrix x, for each row $x_{[i]} = [x_1, \dots, x_k]$ (with $i = 1, \dots, n$), the log-sum-exp (LSE) function calculates

LSE
$$(x_{[i]}) = \log \sum_{j=1}^{k} \exp(x_j + v_j) = m + \log \sum_{j=1}^{k} \exp(x_j + v_j - m)$$

where $m = \max(x_1 + v_1, ..., x_k + v_k)$.

Value

Returns a vector of values of length equal to the number of rows of x.

Author(s)

Luca Scrucca

References

Blanchard P., Higham D. J., Higham N. J. (2021). Accurately computing the log-sum-exp and softmax functions. *IMA Journal of Numerical Analysis*, 41/4:2311–2330. doi:10.1093/imanum/draa038

76 majority Vote

See Also

```
softmax
```

Examples

```
x = matrix(rnorm(15), 5, 3)
v = log(c(0.5, 0.3, 0.2))
logsumexp(x, v)
```

majorityVote

Majority vote

Description

A function to compute the majority vote (some would say plurality) label in a vector of labels, breaking ties at random.

Usage

```
majorityVote(x)
```

Arguments

Х

A vector of values, either numerical or not.

Value

A list with the following components:

table A table of votes for each unique value of x.

ind An integer specifying which unique value of x corresponds to the majority vote.

majority A string specifying the majority vote label.

Author(s)

L. Scrucca

```
x <- c("A", "C", "A", "B", "C", "B", "A")
majorityVote(x)</pre>
```

map 77

m	a	r

Classification given Probabilities

Description

Converts a matrix in which each row sums to 1 to an integer vector specifying for each row the column index of the maximum.

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.

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, aT0b and bT0a which are themselves lists. The aT0b 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

```
classError, table
```

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

Model-based clustering based on parameterized finite Gaussian mixture models. Models are estimated by EM algorithm initialized by hierarchical model-based agglomerative clustering. The optimal model is then selected according to BIC.

Usage

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

Arguments

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

are not allowed. If a matrix or data frame, rows correspond to observations (n)

and columns correspond to variables (d).

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.

A vector of character strings indicating the models to be fitted in the EM phase of clustering. The default is:

• for univariate data (d = 1): c("E", "V")

• for multivariate data (n > d): all the models available in mclust.options("emModelNames")

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

The help file for mclustModelNames describes the available models.

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

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

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.

and data transformation set by mclust.options("hcUse").

For multivariate data, the default is to compute a hierarchical agglomerative clustering tree by applying function hc with model specified by mclust.options("hcModelName"),

All the input or a subset as indicated by the subset argument is used for initial clustering.

The hierarchical clustering results are then used to start the EM algorithm from a given partition.

For univariate data, the default is to use quantiles to start the EM algorithm. However, hierarchical clustering could also be used by calling hc with model specified as "V" or "E".

subset A logical or numeric vector specifying a subset of the data to be used in the initial hierarchical clustering phase. No subset is used unless the number of observations exceeds the value specified by mclust.options("subset"),

modelNames

prior

control

which by default is set to 2000 (see mclust.options). Note that in this case to guarantee exact reproducibility of results a seed must be specified (see set.seed).

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 al-

ready 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.

verbose A logical controlling if a text progress bar is displayed during the fitting proce-

dure. By default is TRUE if the session is interactive, and FALSE otherwise.

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

Value

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.

loglik The log-likelihood corresponding to the optimal BIC.

df The number of estimated parameters.
bic BIC value of the selected model.
icl ICL value of the selected model.

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

to NULL (see hypvol).

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

Scrucca L., Fraley C., Murphy T. B. and Raftery A. E. (2023) *Model-Based Clustering, Classification, and Density Estimation Using mclust in R*. Chapman & Hall/CRC, ISBN: 978-1032234953, https://mclust-org.github.io/book/

Scrucca L., Fop M., Murphy T. B. and Raftery A. E. (2016) mclust 5: clustering, classification and density estimation using Gaussian finite mixture models, *The R Journal*, 8/1, pp. 289-317.

Fraley C. and Raftery A. E. (2002) Model-based clustering, discriminant analysis and density estimation, *Journal of the American Statistical Association*, 97/458, pp. 611-631.

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

 $summary. \\ Mclust, plot. \\ Mclust, priorControl, emControl, hc, mclustBIC, mclustModelNames, \\ mclust. \\ options$

```
mod1 <- Mclust(iris[,1:4])</pre>
summary(mod1)
mod2 <- Mclust(iris[,1:4], G = 3)
summary(mod2, parameters = TRUE)
# Using prior
mod3 <- Mclust(iris[,1:4], prior = priorControl())</pre>
summary(mod3)
mod4 <- Mclust(iris[,1:4], prior = priorControl(functionName="defaultPrior", shrinkage=0.1))</pre>
summary(mod4)
# Clustering of faithful data with some artificial noise added
nNoise <- 100
set.seed(0) # to make it reproducible
Noise <- apply(faithful, 2, function(x)
              runif(nNoise, min = min(x)-.1, max = max(x)+.1))
data <- rbind(faithful, Noise)</pre>
plot(faithful)
points(Noise, pch = 20, cex = 0.5, col = "lightgrey")
set.seed(0)
```

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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.

See Also

deprecated

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 or retrieving default values used by 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.

hcModelName A character string specifying the multivariate model to be used in model-based agglomerative hierarchical clustering for initialization of EM algorithm.

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 (default).

hcUse A character string specifying the type of input variables/transformation to be used in model-based agglomerative hierarchical clustering for initialization of EM algorithm.

Possible values are:

"VARS" original variables;

"STD" standardized variables (centered and scaled);

"SPH" sphered variables (centered, scaled and 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 (default);

"RND" no transformation is applied but a random hierarchical structure is returned (see hcRandomPairs).

For further details see Scrucca and Raftery (2015), Scrucca et al. (2016).

- subset A value specifying the maximal sample size to be used in the model-based hierarchical clustering to start the EM algorithm. If data sample size exceeds this value, a random sample is drawn of size specified by subset.
- fillEllipses A logical value specifying whether or not to fill with transparent colors ellipses corresponding to the within-cluster covariances in case of "classification" plot for 'Mclust' objects, or "scatterplot" graphs for 'MclustDA' objects.
- 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.

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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.

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

Scrucca L. and Raftery A. E. (2015) Improved initialisation of model-based clustering using Gaussian hierarchical partitions. *Advances in Data Analysis and Classification*, 9/4, pp. 447-460.

Scrucca L., Fop M., Murphy T. B. and Raftery A. E. (2016) mclust 5: clustering, classification and density estimation using Gaussian finite mixture models, *The R Journal*, 8/1, pp. 289-317.

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\")")
```

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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

Arguments

data

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

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.

Z

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.

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.

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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 options: "classification" (default), "density", "error", "uncertainty".
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, ylab	An argument specifying a label for the axes.
xlim, ylim	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.

Value

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.

See Also

```
mclust2Dplot, clPairs, coordProj
```

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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), "error", "uncertainty".
addEllipses	A logical indicating whether or not to add ellipses with axes corresponding to the within-cluster covariances.
fillEllipses	A logical specifying whether or not to fill ellipses with transparent colors when ${\tt addEllipses} = {\tt TRUE}.$
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.

Value

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

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See Also

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

Examples

```
faithfulModel <- Mclust(faithful)</pre>
mclust2Dplot(faithful, parameters=faithfulModel$parameters,
             z=faithfulModel$z, what = "classification", main = TRUE)
mclust2Dplot(faithful, parameters=faithfulModel$parameters,
             z=faithfulModel$z, what = "uncertainty", main = TRUE)
```

mclustBIC

BIC for Model-Based Clustering

Description

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

Usage

```
mclustBIC(data, G = NULL, modelNames = NULL,
          prior = NULL, control = emControl(),
          initialization = list(hcPairs = NULL,
                                subset = NULL,
                                noise = NULL),
          Vinv = NULL, warn = mclust.options("warn"),
          x = NULL, verbose = interactive(),
          ...)
```

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.

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.

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

The default is:

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> mclust.options("emModelNames") for multivariate data (n > d)c("EII", "VII", "EEI", "EVI", "VEI", "VVI") the spherical and diagonal models for multivariate data ($n \le d$)

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 agglomerative clustering tree by applying function hc with model specified by mclust.options("hcModelName"), and data transformation set by mclust.options("hcUse").

All the input or a subset as indicated by the subset argument is used for initial clustering.

The hierarchical clustering results are then used to start the EM algorithm from a given partition.

For univariate data, the default is to use quantiles to start the EM algorithm. However, hierarchical clustering could also be used by calling hc with model specified as "V" or "E".

subset A logical or numeric vector specifying a subset of the data to be used in the initial hierarchical clustering phase. By default no subset is used unless the number of observations exceeds the value specified by mclust.options("subset"). The subset argument is ignored if hcPairs are provided. Note that to guarantee exact reproducibility of results a seed must be specified (see set.seed).

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.

verbose

A logical controlling if a text progress bar is displayed during the fitting procedure. By default is TRUE if the session is interactive, and FALSE otherwise.

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

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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.

See Also

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

```
irisBIC <- mclustBIC(iris[,-5])</pre>
irisBIC
plot(irisBIC)
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)
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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Description

Update the BIC (Bayesian Information Criterion) for parameterized Gaussian mixture models by taking the best from BIC results as returned by mclustBIC.

Usage

```
mclustBICupdate(BIC, ...)
```

Arguments

BIC Object of class 'mclustBIC' containing the BIC values as returned by a call to mclustBIC.

... Further objects of class 'mclustBIC' to be merged.

Value

An object of class 'mclustBIC' containing the best values obtained from merging the input arguments. Attributes are also updated according to the best BIC found, so calling Mclust on the resulting ouput will return the corresponding best model (see example).

See Also

```
mclustBIC, Mclust.
```

93 MclustBootstrap

MclustBootstrap 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

```
MclustBootstrap(object, nboot = 999,
                type = c("bs", "wlbs", "pb", "jk"),
                alpha = 1, max.nonfit = 10*nboot,
                verbose = interactive(), ...)
```

Arg

guments	
object	An object of class 'Mclust' or 'densityMclust' providing an estimated Gaussian 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
	"pb" parametric bootstrap
	"jk" jackknife
alpha	A numerical value used when type = "wlbs" to generate weights from a Dirichlet(alpha,, alpha) distribution. By default alpha = 1, so weights are generated from a uniform distribution on the simplex.
max.nonfit	The maximum number of non-estimable models allowed.
verbose	A logical controlling if a text progress bar is displayed during the resampling procedure. By default is TRUE if the session is interactive, and FALSE otherwise.
	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 bootstrap 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.

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Value

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

n The number of observations in the data.

d The dimension of the data.

G A value specifying the number of mixture components.

modelName A character string specifying the mixture model covariances parameterisation

(see mclustModelNames).

parameters A list of estimated parameters for the mixture components with the following

components:

pro a vector of mixing proportions.

mean a matrix of means for each component.

variance an array of covariance matrices for each component.

nboot The number of bootstrap replications if type = "bs" or type = "wlbs". The

sample size if type = "jk".

type The type of resampling approach used.

nonfit The number of resamples that did not convergence during the procedure.

pro A matrix of dimension (nboot x G) containing the bootstrap distribution for the

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.

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

containing the bootstrap distribution for the component covariances.

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.

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.MclustBootstrap, plot.MclustBootstrap, Mclust, densityMclust.

```
data(diabetes)
X <- diabetes[,-1]
modClust <- Mclust(X)
bootClust <- MclustBootstrap(modClust)
summary(bootClust, what = "se")
summary(bootClust, what = "ci")</pre>
```

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```
data(acidity)
modDens <- densityMclust(acidity, plot = FALSE)
modDens <- MclustBootstrap(modDens)
summary(modDens, what = "se")
summary(modDens, what = "ci")</pre>
```

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 controlling if a text progress bar is displayed during the bootstrap procedure. By default is TRUE if the session is interactive, and FALSE otherwise.
• • •	Further arguments passed to or from other methods. In particular, see the optional arguments in mclustBIC.
x	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.

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_{h}^{*} = 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.

boot 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.

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See Also

```
mclustBIC, mclustICL, Mclust
```

Examples

```
data(faithful)
faithful.boot = mclustBootstrapLRT(faithful, model = "VVV")
faithful.boot
plot(faithful.boot, G = 1)
plot(faithful.boot, G = 2)
```

MclustDA

MclustDA discriminant analysis

Description

Discriminant analysis based on Gaussian finite mixture modeling.

Usage

Arguments

data A data frame or matrix giving the training data.

class A vector giving the known class labels (either a numerical value or a character

string) for the observations in the training data.

G 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.

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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.

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 values for EM.

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.

verbose A logical controlling if a text progress bar is displayed during the fitting proce-

dure. By default is TRUE if the session is interactive, and FALSE otherwise.

... 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.

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Author(s)

Luca Scrucca

References

Scrucca L., Fraley C., Murphy T. B. and Raftery A. E. (2023) *Model-Based Clustering, Classification, and Density Estimation Using mclust in R*. Chapman & Hall/CRC, ISBN: 978-1032234953, https://mclust-org.github.io/book/

Scrucca L., Fop M., Murphy T. B. and Raftery A. E. (2016) mclust 5: clustering, classification and density estimation using Gaussian finite mixture models, *The R Journal*, 8/1, pp. 289-317.

Fraley C. and Raftery A. E. (2002) Model-based clustering, discriminant analysis and density estimation, *Journal of the American Statistical Association*, 97/458, pp. 611-631.

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

See Also

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

```
odd \leftarrow seg(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)
```

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```
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, 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])
```

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Description

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

Usage

Arguments

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

tively, Mclust or MclustDA.

1 ambda A tuning parameter in the range [0,1] as described in Scrucca (2014). The direc-

tions that mostly separate the estimated clusters or classes are recovered using the default value 1. Users can set this parameter to balance the relative importance of information derived from cluster/class means and covariances. For instance, a value of 0.5 gives equal importance to differences in means and co-

variances among clusters/classes.

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.

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, 2014).

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.

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The data matrix. Х

Sigma The covariance matrix of the data.

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

A matrix of means for each mixture component. mu

An array of covariance matrices for each mixture component. sigma

pro The estimated prior for each mixture component.

The kernel matrix. lambda The tuning parameter.

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

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

matrix, ordered according to the eigenvalues.

The basis of the estimated dimension reduction subspace. basis

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.

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

reduction subspace.

Author(s)

Luca Scrucca

References

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

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])</pre>
summary(mod)
```

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```
dr <- MclustDR(mod)</pre>
summary(dr)
plot(dr, what = "scatterplot")
plot(dr, what = "evalues")
dr <- MclustDR(mod, lambda = 0.5)</pre>
summary(dr)
plot(dr, what = "scatterplot")
plot(dr, what = "evalues")
# classification
data(banknote)
da <- MclustDA(banknote[,2:7], banknote$Status, modelType = "EDDA")</pre>
dr <- MclustDR(da)</pre>
summary(dr)
da <- MclustDA(banknote[,2:7], banknote$Status)</pre>
dr <- MclustDR(da)</pre>
summary(dr)
```

MclustDRsubsel

Subset selection for GMMDR directions based on BIC

Description

Implements a subset selection method for selecting the relevant directions spanning the dimension reduction subspace for visualizing the clustering or classification structure obtained from a finite mixture of Gaussian densities.

Usage

Arguments

object	An object of class 'MclustDR' resulting from a call to MclustDR.
G	An integer vector specifying the numbers of mixture components or clusters.
modelNames	A vector of character strings indicating the models to be fitted. See mclustModelNames for a description of the available models.
	Further arguments passed through Mclust or MclustDA.

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bic.stop A criterion to terminate the search. If maximal BIC difference is less than

bic.stop then the algorithm stops.

Two tipical values are:

0: algorithm stops when the BIC difference becomes negative (default);

-Inf: algorithm continues until all directions have been selected.

bic.cutoff A value specifying how to select simplest "best" model within bic.cutoff from

the maximum value achieved. Setting this to 0 (default) simply select the model

with the largest BIC difference.

mindir An integer value specifying the minimum number of directions to be estimated.

verbose A logical or integer value specifying if and how much detailed information

should be reported during the iterations of the algorithm.

Possible values are:

0 or FALSE: no trace info is shown;

1 or TRUE: a trace info is shown at each step of the search;

2: a more detailed trace info is is shown.

Details

The GMMDR 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. This is implemented in MclustDR.

The MclustDRsubsel function implements the greedy forward search algorithm discussed in Scrucca (2010) to prune the set of all GMMDR directions. The criterion used to select the relevant directions is based on the BIC difference between a clustering model and a model in which the feature proposal has no clustering relevance. The steps are the following:

- 1. Select the first feature to be the one which maximizes the BIC difference between the best clustering model and the model which assumes no clustering, i.e. a single component.
- 2. Select the next feature amongst those not previously included, to be the one which maximizes the BIC difference.
- 3. Iterate the previous step until all the BIC differences for the inclusion of a feature become less than bic.stop.

At each step, the search over the model space is performed with respect to the model parametrisation and the number of clusters.

Value

An object of class 'MclustDRsubsel' which inherits from 'MclustDR', so it has the same components of the latter plus the following:

basisx The basis of the estimated dimension reduction subspace expressed in terms of

the original variables.

std.basisx The basis of the estimated dimension reduction subspace expressed in terms of

the original variables standardized to have unit standard deviation.

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Author(s)

Luca Scrucca

References

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

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

See Also

MclustDR, Mclust, MclustDA.

```
# clustering
data(crabs, package = "MASS")
x <- crabs[,4:8]
class <- paste(crabs$sp, crabs$sex, sep = "|")</pre>
mod <- Mclust(x)</pre>
table(class, mod$classification)
dr <- MclustDR(mod)</pre>
summary(dr)
plot(dr)
drs <- MclustDRsubsel(dr)</pre>
summary(drs)
table(class, drs$classification)
plot(drs, what = "scatterplot")
plot(drs, what = "pairs")
plot(drs, what = "contour")
plot(drs, what = "boundaries")
plot(drs, what = "evalues")
# classification
data(banknote)
da <- MclustDA(banknote[,2:7], banknote$Status)</pre>
table(banknote$Status, predict(da)$class)
dr <- MclustDR(da)</pre>
summary(dr)
drs <- MclustDRsubsel(dr)</pre>
summary(drs)
table(banknote$Status, predict(drs)$class)
plot(drs, what = "scatterplot")
plot(drs, what = "classification")
plot(drs, what = "boundaries")
```

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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

```
mclustICL(data, G = NULL, modelNames = NULL,
          initialization = list(hcPairs = NULL,
                                 subset = NULL,
                                 noise = NULL),
          x = NULL, \ldots
## S3 method for class 'mclustICL'
summary(object, G, modelNames, ...)
```

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.

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 $(n \le d)$

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 mclustLoglik 107

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.

Scrucca L., Fop M., Murphy T. B. and Raftery A. E. (2016) mclust 5: clustering, classification and density estimation using Gaussian finite mixture models, *The R Journal*, 8/1, pp. 289-317.

See Also

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

Examples

```
data(faithful)
faithful.ICL <- mclustICL(faithful)
faithful.ICL
summary(faithful.ICL)
plot(faithful.ICL)

# compare with
faithful.BIC <- mclustBIC(faithful)
faithful.BIC
plot(faithful.BIC)</pre>
```

mclustLoglik

Log-likelihood from a table of BIC values for parameterized Gaussian mixture models

Description

Compute the maximal log-likelihood from a table of BIC values contained in a 'mclustBIC' object as returned by function mclustBIC.

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Usage

```
mclustLoglik(object, ...)
```

Arguments

object An object of class 'mclustBIC' containing the BIC values as returned by a call

to mclustBIC.

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

Value

An object of class 'mclustLoglik' containing the maximal log-likelihood values for the Gaussian mixture models provided as input.

See Also

```
mclustBIC.
```

Examples

```
BIC <- mclustBIC(iris[,1:4])
mclustLoglik(BIC)</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.

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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 $\frac{1}{2}$

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:

modelName A character string indicating the model. The help file for 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 kth component is the mixing proportion for the kth 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.

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.

z A matrix whose [i,k]th entry is the probability that observation i in the test data

belongs to the *k*th class.

See Also

mclustBIC

Examples

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

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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/unqual 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

"VEE" ellipsoidal, equal shape and orientation (*)

"EVE" ellipsoidal, equal volume 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

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single component

```
"X" univariate normal
"XII" spherical multivariate normal
"XXI" diagonal multivariate normal
"XXX" ellipsoidal multivariate normal
(*) new models in mclust version >= 5.0.0.
```

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).
```

See Also

```
Mclust. mclustBIC
```

Examples

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

MclustSSC

MclustSSC semi-supervised classification

Description

Semi-Supervised classification based on Gaussian finite mixture modeling.

Usage

```
MclustSSC(data, class,
    G = NULL, modelNames = NULL,
    prior = NULL, control = emControl(),
    warn = mclust.options("warn"),
    verbose = interactive(),
    ...)
```

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Arguments

data A data frame or matrix giving the training data.

class A vector giving the known class labels (either a numerical value or a character

string) for the observations in the training data. Observations with unknown

class are encoded as NA.

G An integer value specifying the numbers of mixture components or classes. By

default is set equal to the number of known classes. See the examples below.

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

description in mclustModelNames). See the examples below.

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().

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.

verbose A logical controlling if a text progress bar is displayed during the fitting proce-

dure. By default is TRUE if the session is interactive, and FALSE otherwise.

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

Details

The semi-supervised approach implemented in MclustSSC() is a simple Gaussian mixture model for classification where at the first M-step only observations with known class labels are used for parameters estimation. Then, a standard EM algorithm is used for updating the probability of class membership for unlabelled data while keeping fixed the probabilities for labelled data.

Value

An object of class 'MclustSSC' providing the optimal (according to BIC) Gaussian mixture model for semi-supervised classification.

The details of the output components are as follows:

call The matched call.
data The input data matrix.

class The input class labels (including NAs for unknown labels.

modelName A character string specifying the "best" estimated model.

G A numerical value specifying the number of mixture components or classes of

the "best" estimated model.

n The total number of observations in the data.

d The dimension of the data.

BIC All BIC values.

loglik Log-likelihood for the selected model.

df Number of estimated parameters.

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bic Optimal BIC value.

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.

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).

prior The prior used (if any).

control A list of control parameters used in the EM algorithm.

Author(s)

Luca Scrucca

References

Scrucca L., Fop M., Murphy T. B. and Raftery A. E. (2016) mclust 5: clustering, classification and density estimation using Gaussian finite mixture models, *The R Journal*, 8/1, pp. 289-317.

See Also

summary.MclustSSC, plot.MclustSSC, predict.MclustSSC

Examples

```
# Simulate two overlapping groups
n <- 200
pars <- list(pro = c(0.5, 0.5),
             mean = matrix(c(-1,1), nrow = 2, ncol = 2, byrow = TRUE),
             variance = mclustVariance("EII", d = 2, G = 2))
pars$variance$sigmasq <- 1</pre>
data <- sim("EII", parameters = pars, n = n, seed = 12)
class <- data[,1]</pre>
X <- data[,-1]</pre>
clPairs(X, class, symbols = c(1,2), main = "Full classified data")
# Randomly remove labels
cl <- class; cl[sample(1:n, size = 195)] <- NA</pre>
table(cl, useNA = "ifany")
clPairs(X, ifelse(is.na(cl), 0, class),
        symbols = c(0, 16, 17), colors = c("grey", 4, 2),
        main = "Partially classified data")
```

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```
# Fit semi-supervised classification model
mod_SSC <- MclustSSC(X, cl)</pre>
summary(mod_SSC, parameters = TRUE)
pred_SSC <- predict(mod_SSC)</pre>
table(Predicted = pred_SSC$classification, Actual = class)
ngrid <- 50
xgrid <- seq(-3, 3, length.out = ngrid)</pre>
ygrid <- seq(-4, 4.5, length.out = ngrid)</pre>
xygrid <- expand.grid(xgrid, ygrid)</pre>
pred_SSC <- predict(mod_SSC, newdata = xygrid)</pre>
col <- mclust.options("classPlotColors")[class]</pre>
pch <- class
pch[!is.na(cl)] = ifelse(cl[!is.na(cl)] == 1, 19, 17)
plot(X, pch = pch, col = col)
contour(xgrid, ygrid, matrix(pred_SSC$z[,1], ngrid, ngrid),
        add = TRUE, levels = 0.5, drawlabels = FALSE, lty = 2, lwd = 2)
```

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.

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").

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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.

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

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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. The help file for mclustModelNames describes the available models. A matrix whose [i,k]th entry is an initial estimate of the conditional probability z of the ith observation belonging to the kth 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. A list of control parameters for EM. The defaults are set by the call emControl(). control 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. A logical value indicating whether or not certain warnings (usually related to warn 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:

A character string identifying the model (same as the input argument). modelName The number of observations in the data. The dimension of the data. d G The number of mixture components. A matrix whose [i,k]th entry is the conditional probability of the ith observa-7 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.

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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.

See Also

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

Examples

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

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

Gaussian mixture models

Description

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

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 model. The help file for mclustModelNames

describes the available models.

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.

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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.

Details

This is a more efficient version made available with **mclust** ge6.1 using Fortran code internally.

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 *k*th 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

omponents.

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 estimated mixture model.

bic The BIC value for the estimated mixture model.

Attributes: "info" Information on the iteration.

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

tations.

Author(s)

T. Brendan Murphy, Luca Scrucca

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See Also

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

Examples

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, ...)
meVEE(data, z, prior=NULL, control=emControl(), Vinv=NULL, warn=NULL, ...)
meEVE(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, ...)
```

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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.

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

tion belonging to the *k*th component of the mixture.

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

sumes 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.

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 *k*th 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 *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 compu-

tations.

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See Also

```
em, me, estep, mclust.options
```

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(data, modelName, z, 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.
modelName	A character string indicating the model. The help file for ${\tt mclustModelNames}$ describes the available models.
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. 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 identifying the model (same as the input argument).

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.

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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.

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.

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, ...)
mstepEEE( data, z, prior = NULL, warn = NULL, ...)
```

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```
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. z A matrix whose [i,k]th entry is the conditional probability of the ith observation belonging to the kth component of the mixture. In analyses involving noise, this should not include the conditional probabilities for the noise component. Specification of a conjugate prior on the means and variances. The default asprior 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"). Values controlling termination for models "VEI" and "VEV" that have an itcontrol 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:

mixture model.

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

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

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 kth 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

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

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

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, ...)
```

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 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.

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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.

See Also

```
mvnX, mvnXII, mvnXXI, mvnXXX, mclustModelNames
```

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)
x <- sweep(matrix(rnorm(n*3), n, 3) %*% chol(Sigma),</pre>
           MARGIN = 2, STATS = mu, FUN = "+")
mvn(modelName = "XXX", x)
mvn(modelName = "Ellipsoidal", x)
```

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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.
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 <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.
loglik	The log likelihood for the data in the mixture model.
Attributes:	"WARNING" An appropriate warning if problems are encountered in the computations.

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See Also

mvn, mstepE

Examples

```
n <- 1000
set.seed(0)
x \leftarrow rnorm(n, mean = -1, sd = 2)
mvnX(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 = "+")
mvnXII(x)
set.seed(0)
x \leftarrow sweep(matrix(rnorm(n*3), n, 3) %*% diag(1:3),
            MARGIN = 2, STATS = mu, FUN = "+")
mvnXXI(x)
Sigma <- 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 = "+")
mvnXXX(x)
```

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.

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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.

Value

The number of variance parameters in the corresponding Gaussian mixture model.

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.

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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.

Value

The number of variance parameters in the corresponding Gaussian mixture model.

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

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 <= k).

See Also

```
partconv
```

Examples

```
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>
```

plot.clustCombi 131

lot.clustCombi Plot Combined Clusterings Results
--

Description

Plot combined clusterings results: classifications corresponding to Mclust/BIC and to the hierarchically combined classes, "entropy plots" to help to select a number of classes, and the tree structure obtained from combining mixture components.

Usage

```
## S3 method for class 'clustCombi'
plot(x, what = c("classification", "entropy", "tree"), ...)
```

Arguments

x Object returned by clustCombi function.

what Type of plot.

... Other arguments to be passed to other functions: combiPlot, entPlot, combiTree.

Please see the corresponding documentations.

Value

Classifications are plotted with combiPlot, which relies on the Mclust plot functions. Entropy plots are plotted with entPlot and may help to select a number of classes: please see the article cited in the references. Tree plots are produced by combiTree and graph the tree structure implied by the clusters combining process.

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, combiTree, clustCombi.
```

plot.densityMclust

Examples

```
data(Baudry_etal_2010_JCGS_examples)
## 1D Example
output <- clustCombi(data = 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)
## 2D Example
output <- clustCombi(data = 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)
## 3D Example
output <- clustCombi(data = 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)
```

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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Arguments

x An object of class 'mclustDensity' obtained from a call to densityMclust

function.

data Optional data points.

what The type of graph requested:

"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)

The color to be used to draw the density line in 1-dimension or contours in

higher dimensions.

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.

nlevels An integer, the number of levels to be used in plotting contour densities.

levels A vector of density levels at which to draw the contour lines.

prob A vector of probability levels for computing HDR. Only used if type = "hdr"

and supersede previous nlevels and levels arguments.

gap Distance between subplots, in margin lines, for the matrix of pairwise scatter-

plots.

... Additional arguments passed to surfacePlot.

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.

plot.hc

For two-dimensional data further arguments available are those accepted by the surfacePlot function. In particular, the density can be represented through "contour", "hdr", "image", and "persp" type of graph. For type = "hdr" Highest Density Regions (HDRs) are plotted for probability levels prob. See hdrlevels for details.

For higher dimensionality a scatterplot matrix of pairwise projected densities is drawn.

Author(s)

Luca Scrucca

See Also

densityMclust, surfacePlot, densityMclust.diagnostic, Mclust.

Examples

```
dens <- densityMclust(faithful$waiting, plot = FALSE)</pre>
summary(dens)
summary(dens, parameters = TRUE)
plot(dens, what = "BIC", legendArgs = list(x = "topright"))
plot(dens, what = "density", data = faithful$waiting)
dens <- densityMclust(faithful, plot = FALSE)</pre>
summary(dens)
summary(dens, parameters = TRUE)
plot(dens, what = "density", data = faithful,
     drawlabels = FALSE, points.pch = 20)
plot(dens, what = "density", type = "hdr")
plot(dens, what = "density", type = "hdr", prob = seq(0.1, 0.9, by = 0.1))
plot(dens, what = "density", type = "hdr", data = faithful)
plot(dens, what = "density", type = "persp")
dens <- densityMclust(iris[,1:4], plot = FALSE)</pre>
summary(dens, parameters = TRUE)
plot(dens, what = "density", data = iris[,1:4],
     col = "slategrey", drawlabels = FALSE, nlevels = 7)
plot(dens, what = "density", type = "hdr", data = iris[,1:4])
plot(dens, what = "density", type = "persp", col = grey(0.9))
```

plot.hc

Dendrograms for Model-based Agglomerative Hierarchical Clustering

Description

Display two types for dendrograms for model-based hierarchical clustering objects.

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Usage

```
## S3 method for class 'hc'
plot(x, what=c("loglik","merge"), maxG=NULL, labels=FALSE, hang=0, ...)
```

Arguments

x An object of class 'hc'.

what A character string indicating the type of dendrogram to be displayed.

Possible options are:

"loglik" Distances between dendrogram levels are based on the classification

likelihood.

"merge" Distances between dendrogram levels are uniform, so that levels cor-

respond to the number of clusters.

maxG The maximum number of clusters for the dendrogram. For what = "merge", the

default is the number of clusters in the initial partition. For what = "loglik", the default is the minimum of the maximum number of clusters for which the classification loglikelihood an be computed in most cases, and the maximum number of clusters for which the classification likelihood increases with increas-

ing numbers of clusters.

labels A logical variable indicating whether or not to display leaf (observation) labels

for the dendrogram (row names of the data). These are likely to be useful only if the number of observations in fairly small, since otherwise the labels will be

too crowded to read. The default is not to display the leaf labels.

hang For helust objects, this argument is the fraction of the plot height by which

labels should hang below the rest of the plot. A negative value will cause the labels to hang down from 0. Because model-based hierarchical clustering does not share all of the properties of hclust, the hang argment won't work in many

instances.

... Additional plotting arguments.

Details

The plotting input does not share all of the properties of hclust objects, hence not all plotting arguments associated with hclust can be expected to work here.

Value

A dendrogram is drawn, with distances based on either the classification likelihood or the merge level (number of clusters).

Note

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

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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*.

See Also

hc

Examples

```
data(EuroUnemployment)
hcTree <- hc(modelName = "VVV", data = EuroUnemployment)
plot(hcTree, what = "loglik")
plot(hcTree, what = "loglik", labels = TRUE)
plot(hcTree, what = "loglik", maxG = 5, labels = TRUE)
plot(hcTree, what = "merge")
plot(hcTree, what = "merge", labels = TRUE)
plot(hcTree, what = "merge", labels = TRUE, hang = 0.1)
plot(hcTree, what = "merge", labels = TRUE, hang = -1)
plot(hcTree, what = "merge", labels = TRUE, maxG = 5)</pre>
```

plot.Mclust

Plotting method for Mclust model-based clustering

Description

Plots for model-based clustering results, such as BIC, classification, uncertainty and density.

Usage

```
## S3 method for class 'Mclust'
plot(x, what = c("BIC", "classification", "uncertainty", "density"),
    dimens = NULL, xlab = NULL, ylab = NULL,
    addEllipses = TRUE, main = FALSE, ...)
```

Arguments

x Output from Mclust.

what A string specifying the type of graph requested. Available choices are:

"BIC" plot of BIC values used for choosing the number of clusters.

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"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. Ellipses corresponding to covariances of mixture components are also drawn if addEllipses = TRUE.

"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 data in more than two dimensions a matrix of contours for coordinate projection plot is drawn using specified dimens.

If not specified, in interactive sessions a menu of choices is proposed.

dimens A vector of integers specifying the dimensions of the coordinate projections in

case of "classification", "uncertainty", or "density" plots.

xlab, ylab Optional labels for the x-axis and the y-axis.

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 type of plot drawn.

... Other graphics parameters.

Details

For more flexibility in plotting, use mclust1Dplot, mclust2Dplot, surfacePlot, coordProj, or randProj.

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

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",
    legendArgs = list(x = "bottomright", ncol = 2, cex = 1, inset = 0.01),
    ...)
```

Arguments

x	Output from mclustBIC.
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.
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.
legendArgs	Arguments to pass to the legend function. Set to NULL for no legend.
	Other graphics parameters.

Value

A plot of the BIC values.

See Also

mclustBIC

plot.MclustBootstrap 139

Examples

```
plot(mclustBIC(precip), legendArgs = list(x = "bottomleft"))
plot(mclustBIC(faithful))
plot(mclustBIC(iris[,-5]))
```

 ${\tt plot.MclustBootstrap} \quad \textit{Plot of bootstrap distributions for mixture model parameters}$

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"),
    show.parest = TRUE, show.confint = TRUE,
    hist.col = "grey", hist.border = "lightgrey", breaks = NA,
    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.
show.parest	A logical specifying if the parameter estimate should be drawn as vertical line.
show.confint	A logical specifying if the resampling-based confidence interval should be drawn at the bottom of the graph. Confidence level can be provided as further argument conf.level; see summary.MclustBootstrap.
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	The number of breaks used in histogram to visualize the bootstrap distribution. When NA (default), it is computed as the maximum between the "Sturges" and "Freedman-Diaconis" methods; see nclass.Sturges and nclass.FD.
col, lwd, lty	The color, line width and line type to be used to represent the estimated parameters and confidence intervals.
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.

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Value

A plot for each variable/component of the selected parameters.

See Also

```
MclustBootstrap
```

Examples

```
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")</pre>
```

plot.MclustDA

Plotting method for MclustDA discriminant analysis

Description

Plots for model-based mixture discriminant analysis results, such as scatterplot of training and test data, classification of train and test data, and errors.

Usage

```
## S3 method for class 'MclustDA'
plot(x, what = c("scatterplot", "classification", "train&test", "error"),
    newdata, newclass, dimens = NULL,
    symbols, colors, main = NULL, ...)
```

Arguments

Х

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

what

A string specifying the type of graph requested. Available choices are:

- "scatterplot" = a plot of training data with points marked based on the known classification. Ellipses corresponding to covariances of mixture components are also drawn.
- "classification" = a plot of data with points marked on 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.

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"error" = a plot of training set (or test set if newdata and newclass are provided) with misclassified points marked.

If not specified, in interactive sessions a menu of choices is proposed.

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").

main A logical, a character string, or NULL (default) for the main title. If NULL or

FALSE no title is added to a plot. If TRUE a default title is added identifying the type of plot drawn. If a character string is provided, this is used for the title.

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

Details

For more flexibility in plotting, use mclust1Dplot, mclust2Dplot, surfacePlot, coordProj, or randProj.

Author(s)

Luca Scrucca

See Also

MclustDA, surfacePlot, coordProj, randProj

Examples

```
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]

# common EEE covariance structure (which is essentially equivalent to linear discriminant analysis)
irisMclustDA <- MclustDA(X.train, Class.train, modelType = "EDDA", modelNames = "EEE")
summary(irisMclustDA, parameters = TRUE)
summary(irisMclustDA, newdata = X.test, newclass = Class.test)</pre>
```

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```
# 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")
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)
```

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```
even <- odd + 1
crossMclustDA <- MclustDA(cross[odd,-1], cross[odd,1])
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])</pre>
```

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

Arguments

Y

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.

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"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.

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 classifi-

cation regions.

nlevels The number of levels to use in case what = "contour". asp For scatterplots the y/x aspect ratio, see plot.window.

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

Author(s)

Luca Scrucca

References

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

See Also

MclustDR

Examples

```
mod <- Mclust(iris[,1:4], G = 3)
dr <- MclustDR(mod, lambda = 0.5)
plot(dr, what = "evalues")</pre>
```

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```
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", dimens = 2)
data(banknote)
da <- MclustDA(banknote[,2:7], banknote$Status, G = 1:3)</pre>
dr <- MclustDR(da)</pre>
plot(dr, what = "evalues")
plot(dr, what = "pairs")
plot(dr, what = "contour")
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.

See Also

mclustICL

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Examples

```
data(faithful)
faithful.ICL = mclustICL(faithful)
plot(faithful.ICL)
```

plot.MclustSSC

Plotting method for MclustSSC semi-supervised classification

Description

Plots for semi-supervised classification based on Gaussian finite mixture models.

Usage

```
## S3 method for class 'MclustSSC'
plot(x, what = c("BIC", "classification", "uncertainty"), ...)
```

Arguments

x An object of class 'MclustSSC' resulting from a call to MclustSSC.

what A string specifying the type of graph requested. Available choices are:

"BIC" = plot of BIC values used for model selection, i.e. for choosing the model class covariances.

"classification" = a plot of data with points marked based on the known and the predicted classification.

"uncertainty" = a plot of classification uncertainty.

If not specified, in interactive sessions a menu of choices is proposed.

further arguments passed to or from other methods. See plot.Mclust.

Author(s)

Luca Scrucca

See Also

MclustSSC

predict.densityMclust 147

Examples

```
X <- iris[,1:4]</pre>
class <- iris$Species</pre>
# randomly remove class labels
set.seed(123)
class[sample(1:length(class), size = 120)] <- NA</pre>
table(class, useNA = "ifany")
clPairs(X, ifelse(is.na(class), 0, class),
        symbols = c(0, 16, 17, 18), colors = c("grey", 4, 2, 3),
        main = "Partially classified data")
# Fit semi-supervised classification model
mod_SSC <- MclustSSC(X, class)</pre>
summary(mod_SSC, parameters = TRUE)
pred_SSC <- predict(mod_SSC)</pre>
table(Predicted = pred_SSC$classification, Actual = class, useNA = "ifany")
plot(mod_SSC, what = "BIC")
plot(mod_SSC, what = "classification")
plot(mod_SSC, what = "uncertainty")
```

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", "z"), logarithm = FALSE, ...)
```

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); "z" returns a matrix of conditional probabilities of each data point to belong to a mixture component.
logarithm	A logical value indicating whether or not the logarithm of the density or component densities should be returned.
	further arguments passed to or from other methods.

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Value

Returns a vector or a matrix of densities evaluated at newdata depending on the argument what (see above).

Author(s)

Luca Scrucca

See Also

Mclust.

Examples

```
x <- faithful$waiting
dens <- densityMclust(x, plot = FALSE)
x0 <- seq(50, 100, by = 10)
d0 <- predict(dens, x0)
plot(dens, what = "density")
points(x0, d0, pch = 20)</pre>
```

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 *k*th cluster.

predict.MclustDA 149

Author(s)

Luca Scrucca

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, prop = object$prop, ...)
```

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.

prop the class proportions or prior class probabilities to belong to each class; by de-

fault, this is set at the class 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

See Also

MclustDA.

Examples

```
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</pre>
```

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.

```
## S3 method for class 'MclustDR'
predict(object, dim = 1:object$numdir, newdata, eval.points, ...)
```

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Arguments

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

dim the dimensions of the reduced subspace used for prediction.

newdata a data frame or matrix giving the data. If missing the data obtained from the call

to MclustDR are used.

eval.points a data frame or matrix giving the data projected on the reduced subspace. If

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.

z 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.

See Also

MclustDR.

```
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)
```

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predict.MclustSSC	Classification of multivariate observations by semi-supervised Gaus-
	sian finite mixtures

Description

Classify multivariate observations based on Gaussian finite mixture models estimated by MclustSSC.

Usage

```
## S3 method for class 'MclustSSC'
predict(object, newdata, ...)
```

Arguments

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

newdata a data frame or matrix giving the data. If missing the train data obtained from

the call to MclustSSC are classified.

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

Value

Returns a list of with the following components:

classification a factor of predicted class labels for newdata.

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

Author(s)

Luca Scrucca

See Also

MclustSSC.

priorControl 153

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.

References

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

```
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>
```

randomOrthogonalMatrix

Random orthogonal matrix

Description

Generate a random orthogonal basis matrix of dimension (nrowxncol) using the method in Heiberger (1978).

Usage

```
randomOrthogonalMatrix(nrow, ncol, n = nrow, d = ncol, seed = NULL)
```

Arguments

nrow	the number of rows of the resulting orthogonal matrix.
ncol	the number of columns of the resulting orthogonal matrix.
n	deprecated. See nrow above.
d	deprecated. See ncol above.
seed	an optional integer argument to use in set.seed() for reproducibility. By default the current seed will be used. Reproducibility can also be achieved by calling set.seed() before calling this function.

Details

The use of arguments n and d is deprecated and they will be removed in the future.

Value

An orthogonal matrix of dimension nrowxncol such that each column is orthogonal to the other and has unit length. Because of the latter, it is also called orthonormal.

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References

Heiberger R. (1978) Generation of random orthogonal matrices. *Journal of the Royal Statistical Society. Series C (Applied Statistics)*, 27(2), 199-206.

See Also

```
coordProj
```

Examples

```
B <- randomOrthogonalMatrix(10,3)
zapsmall(crossprod(B))</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.

seeds

An integer value or a vector of integer values to be used as seed for random number generation. If multiple values are provided, then each seed should produce a different projection. By default, a single seed is drawn randomnly, so each call of randProj() produces different projections.

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.

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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 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. 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. A numeric vector of values in (0,1) giving the uncertainty of each data point. If uncertainty present argument z will be ignored. Choose from one of the following three options: "classification" (default), what "error", "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).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. fillEllipses A logical specifying whether or not to fill ellipses with transparent colors when addEllipses = TRUE. 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"). A logical variable indicating whether or not the two chosen dimensions should scale be plotted on the same scale, and thus preserve the shape of the distribution. Default: scale=FALSE Optional arguments specifying bounds for the ordinate, abscissa of the plot. This xlim, ylim may be useful for when comparing plots. xlab, ylab Optional arguments specifying the labels for, respectively, the horizontal and vertical axis. A numerical value specifying the size of the plotting symbols. The default value cex 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 ".".

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Main A logical variable or NULL indicating whether or not to add a title to the plot identifying the dimensions used.

... Other graphics parameters.

Value

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.

The function also returns an invisible list with components basis, the randomnly generated basis of the projection subspace, data, a matrix of projected data, and mu and sigma the component parameters transformed to the projection subspace.

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.

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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.

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.

See Also

decomp2sigma

Examples

```
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>
```

sim

Simulate from Parameterized MVN Mixture Models

Description

Simulate data from parameterized MVN mixture models.

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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 simulation.

See Also

```
simE, ..., simVVV, Mclust, mstep, do.call
```

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```
do.call("sim", irisModel) # alternative call
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)
 irisModel3$n <- NULL
 irisSim3 \leftarrow do.call("sim", c(list(n=500, seed=1), irisModel3)) # alternative call
clPairs(irisSim3[,-1], cl = irisSim3[,1])
```

simE

Simulate from a Parameterized MVN Mixture Model

Description

Simulate data from a parameterized MVN mixture model.

```
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, ...)
```

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```
simEEE(parameters, n, seed = NULL, ...)
simVEE(parameters, n, seed = NULL, ...)
simEVE(parameters, n, seed = NULL, ...)
simVVE(parameters, n, seed = NULL, ...)
simEEV(parameters, n, seed = NULL, ...)
simVEV(parameters, n, seed = NULL, ...)
simEVV(parameters, n, seed = NULL, ...)
simVVV(parameters, n, seed = NULL, ...)
```

Arguments

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 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 simulation.

See Also

```
sim, Mclust, mstepE, mclustVariance.
```

Examples

```
d <- 2
```

G <- 2

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softmax

Softmax function

Description

Efficient implementation (via Fortran) of the softmax (aka multinomial logistic) function converting a set of numerical values to probabilities summing to 1.

Usage

```
softmax(x, v = NULL)
```

Arguments

a matrix of dimension $n \times k$ of numerical values. If a vector is provided, it is converted to a single-row matrix.

v an optional vector of length k of numerical values to be added to each row of x matrix. If not provided, a vector of zeros is used.

Details

Given the matrix x, for each row $x_{[i]} = [x_1, \dots, x_k]$ (with $i = 1, \dots, n$), the softmax function calculates

softmax
$$(x_{[i]})_j = \frac{\exp(x_j + v_j)}{\sum_{l=1}^k \exp(x_l + v_l)}$$
 for $j = 1, ..., k$

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Value

Returns a matrix of the same dimension as x with values in the range (0, 1) that sum to 1 along the rows

Author(s)

Luca Scrucca

References

Blanchard P., Higham D. J., Higham N. J. (2021). Accurately computing the log-sum-exp and softmax functions. *IMA Journal of Numerical Analysis*, 41/4:2311–2330. doi:10.1093/imanum/draa038

See Also

logsumexp

Examples

```
x = matrix(rnorm(15), 5, 3)
v = log(c(0.5, 0.3, 0.2))
(z = softmax(x, v))
rowSums(z)
```

summary.Mclust

Summarizing Gaussian Finite Mixture Model Fits

Description

Summary method for class "Mclust".

Usage

```
## S3 method for class 'Mclust'
summary(object, classification = TRUE, parameters = 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.

classification Logical; if TRUE a table of MAP classification/clustering of observations is printed.

parameters Logical; if TRUE, the parameters of mixture components are printed.

digits The number of significant digits to use when printing.

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

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Author(s)

Luca Scrucca

See Also

```
Mclust, densityMclust.
```

Examples

```
mod1 = Mclust(iris[,1:4])
summary(mod1)
summary(mod1, parameters = TRUE, classification = FALSE)
mod2 = densityMclust(faithful, plot = FALSE)
summary(mod2)
summary(mod2, parameters = 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.

summary.mclustBIC 165

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.

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.

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", "ave"), 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; "ave" for the averages.
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.

See Also

MclustBootstrap.

```
data(diabetes)
X = diabetes[,-1]
modClust = Mclust(X)
bootClust = MclustBootstrap(modClust)
summary(bootClust, what = "se")
summary(bootClust, what = "ci")

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

summary.MclustDA 167

· ·	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	$An \ object \ of \ class \ 's ummary. \ MclustDA', usually, a \ result \ of \ a \ call \ to \ summary. \ MclustDA.$
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

See Also

```
MclustDA, plot.MclustDA.
```

```
mod = MclustDA(data = iris[,1:4], class = iris$Species)
summary(mod)
summary(mod, parameters = TRUE)
```

summary.MclustSSC

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

See Also

MclustDR, plot.MclustDR

summary.MclustSSC	Summarizing semi-supervised classification model based on Gaussian finite mixtures
	finite mixtures

Description

Summary method for class "MclustSSC".

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Usage

```
## S3 method for class 'MclustSSC'
summary(object, parameters = FALSE, ...)
## S3 method for class 'summary.MclustSSC'
print(x, digits = getOption("digits"), ...)
```

Arguments

object An object of class 'MclustSSC' resulting from a call to MclustSSC.

x An object of class 'summary.MclustSSC', usually, a result of a call to summary.MclustSSC.

parameters Logical; if TRUE, the parameters of mixture components are printed.

digits The number of significant digits to use when printing.
... Further arguments passed to or from other methods.

Value

The function summary. MclustSSC computes and returns a list of summary statistics of the estimated MclustSSC model for semi-supervised classification.

Author(s)

Luca Scrucca

See Also

MclustSSC, plot.MclustSSC.

surfacePlot

Density or uncertainty surface for bivariate mixtures

Description

Plots a density or uncertainty surface given bivariate data and parameters of a MVN mixture model for the data.

```
surfacePlot(data, parameters,
    what = c("density", "uncertainty"),
    type = c("contour", "hdr", "image", "persp"),
    transformation = c("none", "log", "sqrt"),
    grid = 200, nlevels = 11, levels = NULL,
    prob = c(0.25, 0.5, 0.75),
    col = gray(0.5),
    col.palette = function(...) hcl.colors(..., "blues", rev = TRUE),
    hdr.palette = blue2grey.colors,
```

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```
xlim = NULL, ylim = NULL, xlab = NULL, ylab = NULL,
main = FALSE, scale = FALSE, swapAxes = FALSE,
verbose = FALSE, ...)
```

Arguments

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.

what Choose from one of the following options: "density" (default), "uncertainty"

indicating what to plot.

type Choose from one of the following three options: "contour" (default), "hdr",

"image", and "persp" indicating the plot type.

 $transformation \quad Choose from one of the following three options: "none" (default), "log", "sqrt" \\$

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.

prob A vector of probability levels for computing HDR. Only used if type = "hdr"

and supersede previous nlevels and levels arguments.

col A string specifying the colour to be used for type = "contour" and type =

"persp" plots.

col.palette A function which defines a palette of colours to be used for type = "image"

plots.

hdr.palette A function which defines a palette of colours to be used for type = "hdr" plots.

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.

main A logical variable or NULL indicating whether or not to add a title to the plot

identifying the dimensions used.

scale A logical variable indicating whether or not the two dimensions should be plot-

ted on the same scale, and thus preserve the shape of the distribution. The default

is not to scale.

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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.

Details

For an image plot, a color scheme may need to be selected on the display device in order to view the plot.

Value

A plots showing (a transformation of) the density or uncertainty for the given mixture model and data.

The function also returns 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.

See Also

```
mclust2Dplot
```

Examples

thyroid

UCI 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.

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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

One of several databases in the Thyroid Disease Data Set (new-thyroid.data, new-thyroid.names) of the UCI Machine Learning Repository https://archive.ics.uci.edu/ml/datasets/thyroid+disease. Please note the UCI conditions of use.

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 probablility from EM to a classification in model-based clustering.

```
uncerPlot(z, truth, ...)
```

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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.

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.

```
unmap(classification, groups=NULL, noise=NULL, ...)
```

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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.

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>
```

wdbc

UCI Wisconsin Diagnostic Breast Cancer Data

Description

The data set provides data for 569 patients on 30 features of the cell nuclei obtained from a digitized image of a fine needle aspirate (FNA) of a breast mass. For each patient the cancer was diagnosed as malignant or benign.

```
data(wdbc)
```

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Format

A data frame with 569 observations on the following variables:

ID ID number

Diagnosis cancer diagnosis: M = malignant, B = benign

Radius_mean a numeric vector

Texture_mean a numeric vector

Perimeter_mean a numeric vector

Area_mean a numeric vector

Smoothness_mean a numeric vector

Compactness_mean a numeric vector

Concavity_mean a numeric vector

Nconcave_mean a numeric vector

Symmetry_mean a numeric vector

Fractaldim_mean a numeric vector

Radius_se a numeric vector

Texture_se a numeric vector

Perimeter_se a numeric vector

Area_se a numeric vector

Smoothness_se a numeric vector

Compactness_se a numeric vector

Concavity_se a numeric vector

Nconcave_se a numeric vector

Symmetry_se a numeric vector

Fractaldim_se a numeric vector

 ${\tt Radius_extreme}\ a\ numeric\ vector$

Texture_extreme a numeric vector

Perimeter_extreme a numeric vector

Area_extreme a numeric vector

Smoothness_extreme a numeric vector

Compactness_extreme a numeric vector

Concavity_extreme a numeric vector

Nconcave_extreme a numeric vector

Symmetry_extreme a numeric vector

Fractaldim_extreme a numeric vector

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Details

The recorded features are:

- Radius as mean of distances from center to points on the perimeter
- Texture as standard deviation of gray-scale values
- Perimeter as cell nucleus perimeter
- · Area as cell nucleus area
- Smoothness as local variation in radius lengths
- Compactness as cell nucleus compactness, perimeter^2 / area 1
- Concavity as severity of concave portions of the contour
- Nconcave as number of concave portions of the contour
- Symmetry as cell nucleus shape
- Fractaldim as fractal dimension, "coastline approximation" 1

For each feature the recorded values are computed from each image as <feature_name>_mean, <feature_name>_se, and <feature_name>_extreme, for the mean, the standard error, and the mean of the three largest values.

Source

The Breast Cancer Wisconsin (Diagnostic) Data Set (wdbc.data, wdbc.names) from the UCI Machine Learning Repository https://archive.ics.uci.edu/ml/datasets/Breast+Cancer+Wisconsin+(Diagnostic). Please note the UCI conditions of use.

References

Mangasarian, O. L., Street, W. N., and Wolberg, W. H. (1995) Breast cancer diagnosis and prognosis via linear programming. *Operations Research*, 43(4), pp. 570-577.

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)

References

C. Fraley, A. E. Raftery and R. Wehrens (2005). Incremental model-based clustering for large datasets with small clusters. *Journal of Computational and Graphical Statistics* 14:1:18.

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