Package ‘ContaminatedMixt’

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Description Fits mixtures of multivariate contaminated normal distributions (with eigen-decomposed scale matrices) via the expectation conditional-maximization algorithm under a clustering or classification paradigm. Methods are described in Antonio Punzo, Angelo Mazza, and Paul D McNicholas (2018) <doi:10.18637/jss.v085.i10>.
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**Description**

This package allows to fit, according to the expectation-conditional maximization algorithm, the 14 parsimonious mixtures of multivariate contaminated normal distributions, with eigen-decomposed scale matrices, introduced by Punzo and McNicholas (2016). Model-based clustering and classification scenarios are implemented. Likelihood-based model selection criteria can be adopted to select the parsimonious model and the number of groups.

**Details**

- **Package:** ContaminatedMixt
- **Type:** Package
- **Version:** 1.1
- **Date:** 2016-09-02
- **License:** GNU-2

**Author(s)**

Antonio Punzo, Angelo Mazza, Paul D. McNicholas

Maintainer: Angelo Mazza <a.mazza@unict.it>

**References**


**See Also**

CNmixt
Description

Evaluates the agreement of a given partition with respect to the partition arising from the mixture of multivariate contaminated normal distributions. If the mixture has been fitted for classification purposes, the agreement will be based on the unlabeled observations only.

Usage

agree(object, givgroup, criterion = "BIC")

Arguments

object An object of class ContaminatedMixt
givgroup vector, of the same dimension of the number of observations used to fit the model in object, representing a given partition
criterion an optional character string with the information criterion to consider; supported values are: "AIC", "AICc", "AICu", "AIC3", "AWE", "BIC", "CAIC", "ICL". Default value is "BIC".

Value

A contingency table.

Author(s)

Antonio Punzo, Angelo Mazza, Paul D. McNicholas

References


See Also

ContaminatedMixt-package, CNmixt
**CNmixt**

*Fitting for the Parsimonious Mixtures of Contaminated Normal Distributions*

**Description**

Fits, by using the expectation conditional-maximization (ECM) algorithm, parsimonious mixtures of multivariate contaminated normal distributions (with eigen-decomposed scale matrices) to the given data within a clustering paradigm (default) or classification paradigm. Can be run in parallel. Likelihood-based model selection criteria are used to select the parsimonious model and the number of groups.

**Usage**

```r
CNmixt(X, G, contamination = NULL, model = NULL, initialization = "mixt", alphafix = NULL, alphamin = 0.5, seed = NULL, start.z = NULL, start.v = NULL, start = 0, label = NULL, AICcond = FALSE, iter.max = 1000, threshold = 1.0e-10, parallel = FALSE, eps = 1e-100, verbose = TRUE)
```

```r
CNmixtCV(X, G, contamination = NULL, model = NULL, initialization = "mixt", k = 10, alphafix = NULL, alphamin = 0.5, seed = NULL, start.z = NULL, start.v = NULL, start = 0, label = NULL, iter.max = 1000, threshold = 1.0e-10, parallel = FALSE, eps = 1e-100, verbose = TRUE)
```

**Arguments**

- **X** a dim=c(n, p) matrix such that the n rows correspond to observations and the p columns correspond to variables.
- **G** a vector containing the numbers of groups to be tried.
- **contamination** an optional boolean indicating if the model(s) to be fitted have to be contaminated or not. If NULL, then both types of models are fitted.
- **model** a vector indicating the model(s) to be fitted. In the multivariate case (p > 1), possible values are: "EII", "VII", "EEI", "VEI", "EVI", "VVI", "EEE", "VEE", "EVE", "EEV", "VVE", "VEV", "VVV". If NULL, then all 14 models are fitted. In the univariate case (p = 1), possible values are "E" and "V".
- **initialization** initialization strategy for the ECM algorithm. It can be:
  - "mixt" (default): the initial (n x G) matrix with posterior probabilities of groups membership arises from a preliminary run of mixtures of multivariate normal distributions as fitted by the gpcm() function of the mixture package (see mixture:gpcm for details).
  - "kmeans": the initial (n x G) hard classification matrix arises from a preliminary run of the k-means algorithm;
  - "random.post": the initial (n x G) matrix with posterior probabilities of groups membership is randomly generated;
• "random.clas": the initial \((n \times G)\) classification matrix is randomly generated;
• "manual": the user must specify either the initial \((n \times G)\) classification matrix or the initial \((n \times G)\) matrix with posterior probabilities of groups membership, via the argument `start.z` and, optionally, the initial \((n \times G)\) matrix of posterior probabilities to be a good observation in each group, via the argument `start.v`.

`alphafix` a vector of length \(G\) with the proportion of good observations in each group. If `length(alphafix) != G`, then the first element is replicated \(G\) times. Default value is NULL.

`alphamin` a vector of length \(G\) with the minimum proportion of good observations in each group. If `length(alphamin) != G`, then the first element is replicated \(G\) times. Default value is 0.5.

`seed` the seed for the random number generator, when random initializations are used; if NULL, current seed is not changed. Default value is NULL.

`start.z` initial \(n \times G\) matrix of either soft or hard classification. Default value is NULL.

`start.v` initial \(n \times G\) matrix of posterior probabilities to be a good observation in each group. Default value is a \(n \times G\) matrix of ones.

`start` when `initialization = "mixt"`, initialization used for the `gpcm()` function of the `mixture` package (see `mixture: gpcm` for details).

`label` a vector of integers of length equal to the number of rows of \(X\). It indicates the known group of membership of each observation. Use 0 when membership is not known. Use NULL when membership is unknown for all observations.

`AICcond` When TRUE, the AICcond criterion, an estimate of the predictive ability of a generative model for classification, is computed (Vandewalle et al., 2013).

`iter.max` maximum number of iterations in the ECM algorithm. Default value is 1000.

`threshold` threshold for Aitken’s acceleration procedure. Default value is 1e-03.

`parallel` When TRUE, the package `parallel` is used for parallel computation. When several models are estimated, computational time is reduced. The number of cores to use may be set with the global option `cl.cores`; default value is detected using `detectCores()`.

`eps` an optional scalar. It sets the smallest value for the eigenvalues of the component scale matrices. Default value is 1e-100.

`k` number of equal sized subsamples used in \(k\)-fold cross-validation.

`verbose` write text to the console

**Details**

The multivariate data contained in \(X\) are either clustered or classified using parsimonious mixtures of multivariate contaminated normal distributions with some or all of the 14 parsimonious models described in Punzo and McNicholas (2016). Model specification (via the `model` argument) follows the nomenclature popularized in other packages such as `mixture` and `mclust`. Such a nomenclature refers to the decomposition and constraints on the scale matrix (see Banfield and Raftery, 1993, Celeux and Govaert, 1995 and Punzo and McNicholas, 2016 for details):

\[
\Sigma_g = \lambda_g \Gamma_g \Delta_g \Gamma_g'.
\]
The nomenclature describes (in order) the volume ($\lambda_g$), shape ($\Delta_g$), and orientation ($\Gamma_g$), in terms of "V"ariable, "E"qual, or the "I"dentity matrix. As an example, the string "VEI" would refer to the model where $\Sigma_g = \lambda_g \Delta$. Note that for $G = 1$, several models are equivalent (for example, "EEE" and "VVV"). Thus, for $G = 1$ only one model from each set of equivalent models will be run.

The algorithms detailed in Celeux and Govaert (1995) are considered in the first CM-step of the ECM algorithm to update $\Sigma_g$ for all the models apart from "EVE" and "VVE". For "EVE" and "VVE", majorization-minimization (MM) algorithms (Hunter and Lange, 2000) and accelerated line search algorithms on the Stiefel manifold (Absil, Mahony and Sepulchre, 2009 and Browne and McNicholas, 2014), which are especially preferable in higher dimensions (Browne and McNicholas, 2014), are used to update $\Sigma_g$; the same approach is also adopted in the mixture package for those models.

Starting values are very important to the successful operation of these algorithms and so care must be taken in the interpretation of results. All the initializations considered here provide initial quantities for the first CM-step of the ECM algorithm. The predictive ability of a model for classification may be estimated using the cross-validated error rate, returned by CNmixtCV or through the AIC-cond criterion (Vandewalle et al., 2013).

**Value**

CNmixt returns an object of class ContaminatedMixt. CNmixtCV returns a list with the cross-validated error rate estimated for each model.

**Author(s)**

Antonio Punzo, Angelo Mazza, Paul D. McNicholas

**References**


**See Also**

`ContaminatedMixt-package`

**Examples**

```r
## Note that the example is extremely simplified
## in order to reduce computation time

# Artificial data from an EEI Gaussian mixture with G = 2 components

library("mnormt")
p <- 2
set.seed(12345)
X1 <- rmnorm(n = 200, mean = rep(2, p), varcov = diag(c(5, 0.5)))
X2 <- rmnorm(n = 200, mean = rep(-2, p), varcov = diag(c(5, 0.5)))
noise <- matrix(runif(n = 40, min = -20, max = 20), nrow = 20, ncol = 2)
X <- rbind(X1, X2, noise)

group <- rep(c(1, 2, 3), times = c(200, 200, 20))
plot(X, col = group, pch = c(3, 4, 16)[group], asp = 1, xlab = expression(X[1]),
ylab = expression(X[2]))

# ---------------------- #
# Model-based clustering #
# ---------------------- #

res1 <- CNmixt(X, model = c("EEI", "VVV"), G = 2, parallel = FALSE)
summary(res1)
agree(res1, givgroup = group)
plot(res1, contours = TRUE, asp = 1, xlab = expression(X[1]), ylab = expression(X[2]))

# -------------------------- #
# Model-based classification #
# -------------------------- #

indlab <- sample(1:400, 20)
lab <- rep(0, nrow(X))
lab[indlab] <- group[indlab]
res2 <- CNmixt(X, G = 2, model = "EEI", label = lab)
```
agree(res2, givgroup = group)

---

**CNpredict**

*Cluster Prediction*

**Description**

Cluster prediction for multivariate observations based on uncontaminated/contaminated normal mixture models

**Usage**

```r
CNpredict(newdata, prior, mu, invSigma, eta=NULL, alpha=NULL)
```

**Arguments**

- `newdata`: a dim=c(n, p) matrix representing the coordinates of n new data point(s)
- `object`: an object of class `ContaminatedMixt` resulting from a call to `CNmixt`. When several models have been estimated, `getBestModel` is used to select one of them
- `...`: Options to be passed to `getBestModel`
- `prior`: a vector with length=G, where G is the number of components of the mixture model. Its kth component is the mixing proportion for the kth component
- `mu`: a dim=c(p, G) matrix with mean values for each component of the mixture model
- `invSigma`: an array with dim=c(p, p, G) whose element invSigma[,k] is the inverse covariance matrix for the kth component of the mixture model
- `alpha`: a vector of length=G with the proportions of good observations; it must be a number between 0 and 1. Use NULL for uncontaminated models
- `eta`: a vector of length=G with the degree of contamination; it should be a number greater than 1. Use NULL for uncontaminated models

**Value**

- a vector with group membership

**Author(s)**

Antonio Punzo, Angelo Mazza, Paul D. McNicholas
**References**


**See Also**

*ContaminatedMixt-package*

**Examples**

```r
point <- c(0,0,0)
mu <- c(1,-2,3)
Sigma <- diag(3)
alpha <- 0.8
eta <- 5
f <- dCN(point, mu, Sigma, alpha, eta)
x <- rCN(10, mu, Sigma, alpha, eta)
```

---

**dCN**  
**Multivariate Contaminated Normal Distribution**

**Description**

Probability density function and random number generation for the multivariate contaminated normal distribution.

**Usage**

```r
dCN(x, mu = rep(0,p), Sigma, alpha = 0.99, eta = 1.01)
rCN(n, mu = rep(0,p), Sigma, alpha = 0.99, eta = 1.01)
```

**Arguments**

- `x`  
either a vector of length p or a matrix with p columns, being p = ncol(Sigma), representing the coordinates of the point(s) where the density must be evaluated
- `mu`  
either a vector of length p, representing the mean value, or (except for rCN) a matrix whose rows represent different mean vectors; if it is a matrix, its dimensions must match those of x
- `Sigma`  
a symmetric positive-definite matrix representing the scale matrix of the distribution; a vector of length 1 is also allowed (in this case, p = 1 is set)
- `alpha`  
proportion of good observations; it must be a number between 0 and 1
- `eta`  
the degree of contamination; it should be a number greater than 1
- `n`  
the number of random vectors to be generated
Extractor functions

Value

dCN returns a vector of density values; rCN returns a matrix of \( n \) rows of random vectors

Author(s)

Antonio Punzo, Angelo Mazza, Paul D. McNicholas

References


See Also

ContaminatedMixt-package

Examples

```r
point <- c(0,0,0)
mu <- c(1,-2,3)
Sigma <- diag(3)
alpha <- 0.8
eta <- 5
f <- dCN(point, mu, Sigma, alpha, eta)
x <- rCN(10, mu, Sigma, alpha, eta)
```

Extractor functions Extractors for ContaminatedMixt Class Objects.

Description

These functions extract values from ContaminatedMixt class objects.

Usage

```r
getBestModel(object, criterion = "BIC", G = NULL, model = NULL, contamination = NULL)
getPosterior(object, ...)
getSize(object, ...)
getCluster(object, ...)
getPar(object, ...)
getCV(object)
```
Extractor functions

getIC(object, criteria)
getDetection(object, ...)
whichBest(object, criteria = NULL, G = NULL, model = NULL,
  contamination = NULL)
whichBestCV (object, G=NULL, model=NULL, contamination=NULL)
## S3 method for class 'ContaminatedMixt'
summary(object, criterion = "BIC",
  digits =getOption("digits")-2, ...)
## S3 method for class 'ContaminatedMixt'
print(x, ...)

Arguments

object, x a class ContaminatedMixt object or a class ContaminatedMixt object for
  getCV and whichBestCV.
criterion a string with the information criterion to consider; supported values are: "AIC",
  "AICc", "AICcond", "AICu", "AIC3", "AWE", "BIC", "CAIC", "ICL". Default
  value is "BIC".
criteria a vector of strings with the names of information criteria to consider. If NULL,
  all the supported information criteria are considered.
G an optional vector containing the numbers of groups to consider. If not specified,
  all the estimated models are considered.
model an optional vector of character strings indicating the parsimonious models to
  consider. If not specified, all the estimated models are considered.
contamination an optional boolean indicating if the model(s) to be considered have to be con-
  taminated or not. If NULL, then both types of models are considered.
digits integer used for number formatting.
... additional arguments to be passed to getBestModel (or to whichBest for the
  print method).

Details

When several models have been estimated, these functions consider the best model according to the
information criterion in criterion, among the estimated models having a number of components
among those in G and a parsimonious model among those in model. whichBestCV considers the best
model according to the cross-validated error rates computed by CNmixtCV. getIC provides values
for the information criteria in criteria.

The getBestModel method returns a ContaminatedMixt object containing the best model only,
selected as described above.
m.step  

M-step of the EM algorithm for Parsimonious Normal Mixtures

Description

Carries out the M-step for EM algorithm

Usage

m.step(X, modelname, z, mtol=1e-10, mmax=10)

Arguments

X  
a matrix such that \( n \) rows correspond to observations and \( p \) columns correspond to variables.

modelname  
a three letter sequence indicating the covariance structure. Possible values are: "EII", "VII", "EEI", "VEI", "EV1", "VVE", "EEE", "VEE", "EEV", "EEE", "VVE", "VEV", "EVV", "VVV".

z  
a matrix of weights such that \( n \) rows correspond to observations and \( G \) columns correspond to groups.

mtol  
the convergence criteria for the M-step if an iterative procedure is necessary.

mmax  
the maximum number of iterations for an iterative procedure.

Value

A list of the model parameters with the mu, Sigma, invSigma and px for each group.

Author(s)

Antonio Punzo, Angelo Mazza, Paul D. McNicholas

References


See Also

ContaminatedMixt-package
Examples

point <- c(0,0,0)
mu <- c(1,-2,3)
Sigma <- diag(3)
alpha <- 0.8
eta <- 5
f <- dCN(point, mu, Sigma, alpha, eta)
x <- rCN(10, mu, Sigma, alpha, eta)

pairs.ContaminatedMixt

Scatterplot Matrix for ContaminatedMixt Objects

Description

A matrix of scatterplots, for objects of class ContaminatedMixt, is produced.

Usage

## S3 method for class 'ContaminatedMixt'
pairs(x, criterion = "BIC", ...)

Arguments

x an object of class ContaminatedMixt
criterion an optional character string with the information criterion to consider; supported values are: "AIC", "AICc", "AICu", "AIC3", "AWE", "BIC", "CAIC", "ICL". Default value is "BIC".
... Options to be passed to pairs.

Author(s)

Antonio Punzo, Angelo Mazza, Paul D. McNicholas

See Also

ContaminatedMixt
plot.ContaminatedMixt  Scatterplot for ContaminatedMixt Objects

Description

Scatterplot, with optionally superimposed contours, for objects of class ContaminatedMixt.

Usage

## S3 method for class 'ContaminatedMixt'
plot(x, criterion = "BIC", contours = FALSE, xmargin = 1, ymargin = 2,
     res = 200, levels = seq(.0001,1,by=0.01), ...)

Arguments

- **x**: an object of class ContaminatedMixt
- **criterion**: a string with the information criterion to consider; supported values are: "AIC", "AICc", "AICu", "AIC3", "AWE", "BIC", "CAIC", "ICL". Default value is "BIC".
- **contours**: if TRUE, the contours of the mixture density are superimposed on the plot. Default is FALSE.
- **xmargin**: scalar argument giving the position of the variable to be used on the x-axis.
- **ymargin**: scalar argument giving the position of the variable to be used on the y-axis.
- **res**: scalar argument giving the resolution for the calculation grid required for the contour plot. Default is 200, which results in a $200 \times 200$ grid.
- **levels**: numeric vector giving the levels at which contours should be drawn. Default is to draw a contour in 0.01 steps, starting from the contour of height .0001. This may result in more/less contours than desired depending on the resulting density.
- **...**: Options to be passed to plot.

Author(s)

Antonio Punzo, Angelo Mazza, Paul D. McNicholas

See Also

CNmixt
Description

These data are the results of a chemical analysis of wines grown in the same region in Italy but derived from three different cultivars. The analysis determined the quantities of 13 constituents found in each of the three types of wine: Barolo, Grignolino, Barbera. The data set is used to evaluate the ability of the CNmixt() function in clustering the data assuming unknown their cultivars.

Usage

data(wine)

Format

This data frame contains 178 rows, each corresponding to a different cultivar of wine produced in Piedmont (Italy), and 14 columns. The first column is the type of wine (Type), a factor variable with the following levels: Barolo, Grignolino, Barbera. The variables measured on the three types of wines are the following: Alcohol, Malic acid, Ash, Alcalinity, Magnesium, Phenols, Flavanoids, Nonflavanoids, Proanthocyanins, Color intensity, Hue, OD280.OD315Dilution, Proline. All variables but the label class are continuous.

Details

The original data set comprises 27 variables. Here a subset of 14 variables only has been included.

Source

This dataset is from the UCI machine learning repository and it is available at http://archive.ics.uci.edu/ml/datasets/Wine.

References


See Also

ContaminatedMixt-package, CNmixt

Examples

data("wine")

group <- wine[, 1]
pairs(wine[, -1], cex = 0.6, pch = c(2, 3, 1)[group], col = c(3, 4, 2)[group], gap = 0,
cex.labels = 0.6)

res3 <- CNmixt(wine[, -1], G = 3, model = "EEE", initialization = "random.post",
    seed = 5, parallel = FALSE)
agree(res3, givgroup = group)
pairs(res3, cex = 0.6, gap = 0, cex.labels = 0.6)
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