# Package 'mixture'

January 30, 2024
Type Package
Title Mixture Models for Clustering and Classification
Version 2.1.1
<b>Date</b> 2024-01-29
Maintainer Paul D. McNicholas <mcnicholas@math.mcmaster.ca></mcnicholas@math.mcmaster.ca>
<b>Description</b> An implementation of 14 parsimonious mixture models for model-based clustering or model-based classification. Gaussian, Student's t, generalized hyperbolic, variance-gamma or skew-t mixtures are available. All approaches work with missing data. Celeux and Govaert (1995) <doi:10.1016 0031-3203(94)00125-6="">, Browne and McNicholas (2014) <doi:10.1007 s11634-013-0139-1="">, Browne and McNicholas (2015) <doi:10.1002 cjs.11246="">.</doi:10.1002></doi:10.1007></doi:10.1016>
Repository CRAN
LazyLoad yes
NeedsCompilation yes
License GPL (>= 2)
Imports Rcpp (>= 1.0.2), methods
LinkingTo Rcpp, RcppArmadillo, BH, RcppGSL
<b>Depends</b> R (>= 3.5.0), lattice (>= 0.20)
SystemRequirements GNU GSL
Author Nik Pocuca [aut] ( <a href="https://orcid.org/0000-0001-8365-0751">https://orcid.org/0000-0001-8365-0751</a> ),  Ryan P. Browne [aut] ( <a href="https://orcid.org/0000-0003-4543-0218">https://orcid.org/0000-0003-4543-0218</a> ),  Paul D. McNicholas [aut, cre] ( <a href="https://orcid.org/0000-0002-2482-523X">https://orcid.org/0000-0002-2482-523X</a> )
<b>Date/Publication</b> 2024-01-30 00:20:07 UTC
R topics documented:
ARI

2 ARI

```
MAP......
40
Index
 43
```

ARI

Adjusted Rand Index

# **Description**

Calculates an adjusted for chance Rand index.

#### Usage

```
ARI(x,y)
```

# **Arguments**

x predictor class memberships y true class memberships

#### Author(s)

Nik Pocuca, Ryan P. Browne and Paul D. McNicholas.

Maintainer: Paul D. McNicholas <mcnicholas@math.mcmaster.ca>

```
x <- sample(1:10, size = 100, replace = TRUE)
y <- sample(1:10, size = 100, replace = TRUE)
ARI(x,y)</pre>
```

e\_step 3

e_step Expectation Step
-------------------------

# Description

Calculates the expectation of class memberships, and imputes if missing values for a given dataset.

# Usage

```
e_step(data, model_obj, start=0, nu = 1.0)
```

# Arguments

data	A matrix or data frame such that rows correspond to observations and columns correspond to variables. Note that this function currently only works with multivariate data $p > 1$ .
start	Start values in this context are only used for imputation. Non-missing values have their expectation of class memberships calculated directly. If 0 then the random soft function is used for initialization. If 1 then the random hard function is used for initialization. If 2 then the kmeans function is used for initialization. If is.matrix then matrix is used as an initialization matrix as along as it has non-negative elements. Note: only models with the same number of columns of this matrix will be fit.
model_obj	A gpcm_best, vgpcm_best, stpcm_best, ghpcm_best, and salpcm_best object class.
nu	deterministic annealing for the class membership E-step.

# **Details**

This will only work on a dataset with the same dimension as estimated in the model. e\_step will also work for missing values, provided that there is at least one non-missing entry.

# Value

Returns a list with the following components:

Χ	A matrix of the original dataset plus imputed values if applicable.
origX	A matrix of the original dataset including missing values.
map	A vector of integers indicating the maximum <i>a posteriori</i> classifications for the best model.
z	A matrix giving the raw values upon which map is based.
row_tags	If there were NAs in the original dataset, a vector of indices referencing the row of the imputed vectors is given.

e\_step

#### Author(s)

Nik Pocuca, Ryan P. Browne and Paul D. McNicholas.

Maintainer: Paul D. McNicholas <mcnicholas@math.mcmaster.ca>

#### References

Browne, R.P. and McNicholas, P.D. (2014). Estimating common principal components in high dimensions. *Advances in Data Analysis and Classification* **8**(2), 217-226.

Zhou, H. and Lange, K. (2010). On the bumpy road to the dominant mode. *Scandinavian Journal of Statistics* **37**, 612-631.

Celeux, G., Govaert, G. (1995). Gaussian parsimonious clustering models. *Pattern Recognition* **28**(5), 781-793.

```
## Not run:
# load dataset and perform model search.
data(x2)
data_in <- matrix(x2,ncol = 2)</pre>
mm <- mixture::gpcm(data = data_in,G = 1:7,</pre>
           start = 0,
           veo = FALSE,pprogress=FALSE)
# get best model
best = get_best_model(mm)
# lets try imputing some missing data.
x2NA <- x2
x2NA[5,1] \leftarrow NA
x2NA[140,2] <- NA
x2NA[99,1] <- NA
# calculate expectation
expect <- e_step(data=x2NA,start = 0,nu = 1.0,model_obj = best)</pre>
# plot imputed entries and compare with original
plot(x2,col = "grey")
points(expect\$X[expect\$row\_tags+1,], col = "blue", pch = 20, cex = 2) \ \# \ blue \ are \ imputed \ values.
points(x2[expect$row_tags+1,], col = "red" , pch = 20,cex = 2) # red are original values.
legend(-2,2,legend = c("imputed","original"),col = c("blue","red"),pch = 20)
## End(Not run)
```

get\_best\_model 5

## **Description**

Carries out model-based clustering or classification using some or all of the 14 parsimonious Gaussian clustering models (GPCM).

# Usage

```
get_best_model(gpcm_model)
```

# **Arguments**

gpcm\_model An input of class gpcm.

#### **Details**

Extracts the best model based on BIC.

#### Value

An object of class gpcm\_best is a list with components:

model_type		summarized			

(Covariance structure and number of groups).

model\_obj An internal list containing all parameters returned from the C++ call.

BIC Bayesian Index Criterion (positive scale, bigger is better).

loglik Log liklihood from the estimated model.

Number of a parameters in the mode.

startobject The type of object inputted into start.

G An integer representing the number of groups.

cov\_type A string representing the type of covariance matrix (see 14 models).

status Convergence status of EM algorithm according to Aitken's Acceleration

map A vector of integers indicating the maximum a posteriori classifications for the

best model.

of the imputed vectors is given.

#### Author(s)

Nik Pocuca, Ryan P. Browne and Paul D. McNicholas.

Maintainer: Paul D. McNicholas <mcnicholas@math.mcmaster.ca>

6 ghpcm

#### References

Browne, R.P. and McNicholas, P.D. (2014). Estimating common principal components in high dimensions. *Advances in Data Analysis and Classification* **8**(2), 217-226.

Zhou, H. and Lange, K. (2010). On the bumpy road to the dominant mode. *Scandinavian Journal of Statistics* **37**, 612-631.

Celeux, G., Govaert, G. (1995). Gaussian parsimonious clustering models. *Pattern Recognition* **28**(5), 781-793.

# **Examples**

ghpcm

Generalized Hyperbolic Parsimonious Clustering Models

# **Description**

Carries out model-based clustering or classification using some or all of the 14 parsimonious Generalized Hyperbolic clustering models (GHPCM).

#### Usage

```
ghpcm(data=NULL, G=1:3, mnames=NULL,
start=2, label=NULL,
veo=FALSE, da=c(1.0),
nmax=1000, atol=1e-8, mtol=1e-8, mmax=10, burn=5,
pprogress=FALSE, pwarning=FALSE, stochastic = FALSE, seed=123)
```

#### **Arguments**

data

A matrix or data frame such that rows correspond to observations and columns correspond to variables. Note that this function currently only works with multivariate data p > 1.

G

A sequence of integers giving the number of components to be used.

7 ghpcm

mnames The models (i.e., covariance structures) to be used. If NULL then all 14 are fitted. If 0 then the random soft function is used for initialization. If 1 then the random start hard function is used for initialization. If 2 then the kmeans function is used for initialization. If >2 then multiple random soft starts are used for initialization. If is.matrix then matrix is used as an initialization matrix as along as it has non-negative elements. Note: only models with the same number of columns of this matrix will be fit. label If NULL then the data has no known groups. If is.integer then some of the observations have known groups. If label[i]=k then observation belongs to group k. If label[i]=0 then observation has no known group. See Examples. Stands for "Variables exceed observations". If TRUE then if the number variables veo in the model exceeds the number of observations the model is still fitted. da Stands for Determinstic Annealing. A vector of doubles. The maximum number of iterations each EM algorithm is allowed to use. nmax A number specifying the epsilon value for the convergence criteria used in the atol

EM algorithms. For each algorithm, the criterion is based on the difference between the log-likelihood at an iteration and an asymptotic estimate of the loglikelihood at that iteration. This asymptotic estimate is based on the Aitken acceleration and details are given in the References.

mtol A number specifying the epsilon value for the convergence criteria used in the

M-step in the GEM algorithms.

The maximum number of iterations each M-step is allowed in the GEM algommax

rithms.

The burn in period for imputing data. (Missing observations are removed and a burn

model is estimated seperately before placing an imputation step within the EM.)

pprogress If TRUE print the progress of the function.

pwarning If TRUE print the warnings.

stochastic If TRUE, it will run stochastic E step variant.

The seed for the run, default is 123 seed

#### Details

The data x are either clustered or classified using Generalized Hyperbolic mixture models with some or all of the 14 parsimonious covariance structures described in Celeux & Govaert (1995). The algorithms given by Celeux & Govaert (1995) is used for 12 of the 14 models; the "EVE" and "VVE" models use the algorithms given in Browne & McNicholas (2014). Starting values are very important to the successful operation of these algorithms and so care must be taken in the interpretation of results.

#### Value

An object of class ghpcm is a list with components:

A vector of integers indicating the maximum a posteriori classifications for the map

best model.

8 ghpcm

model\_objs A list of all estimated models with parameters returned from the C++ call.

best\_model A class of vgpcm\_best containing; the number of groups for the best model, the

covariance structure, and Bayesian Information Criterion (BIC) value.

loglik The log-likelihood values from fitting the best model.

z A matrix giving the raw values upon which map is based.

BIC A G by mnames by 3 dimensional array with values pertaining to BIC calcula-

tions. (legacy)

startobject The type of object inputted into start.

gpar A list object for each cluster pertaining to parameters. (legacy)

row\_tags If there were NAs in the original dataset, a vector of indices referencing the row

of the imputed vectors is given.

**Best Model:** An object of class ghpcm\_best is a list with components:

model\_type A string containg summarized information about the type of model estimated

(Covariance structure and number of groups).

model\_obj An internal list containing all parameters returned from the C++ call.

BIC Bayesian Index Criterion (positive scale, bigger is better).

loglik Log liklihood from the estimated model.

nparam Number of a parameters in the mode.

startobject The type of object inputted into start.

G An integer representing the number of groups.

cov\_type A string representing the type of covariance matrix (see 14 models).

status Convergence status of EM algorithm according to Aitken's Acceleration

map A vector of integers indicating the maximum a posteriori classifications for the

best model.

row\_tags If there were NAs in the original dataset, a vector of indices referencing the row

of the imputed vectors is given.

**Internal Objects:** All classes contain an internal list called model\_obj or model\_objs with the following components:

zigs a posteori matrix

G An integer representing the number of groups.

sigs A vector of covariance matrices for each group

mus A vector of location vectors for each group

alphas A vector containg skewness vectors for each group

gammas A vector containing estimated gamma parameters for each group

## Note

Dedicated print, plot and summary functions are available for objects of class ghpcm.

#### Author(s)

Nik Pocuca, Ryan P. Browne and Paul D. McNicholas.

Maintainer: Paul D. McNicholas <mcnicholas@math.mcmaster.ca>

## References

McNicholas, P.D. (2016), *Mixture Model-Based Classification*. Boca Raton: Chapman & Hall/CRC Press

Browne, R.P. and McNicholas, P.D. (2014). Estimating common principal components in high dimensions. *Advances in Data Analysis and Classification* **8**(2), 217-226.

Browne, R.P. and McNicholas, P.D. (2015), 'A mixture of generalized hyperbolic distributions', Canadian Journal of Statistics 43(2), 176-198.

Zhou, H. and Lange, K. (2010). On the bumpy road to the dominant mode. *Scandinavian Journal of Statistics* **37**, 612-631.

Celeux, G., Govaert, G. (1995). Gaussian parsimonious clustering models. *Pattern Recognition* **28**(5), 781-793.

## **Examples**

```
## Not run:
data("sx2")

### use random soft initializations.
ax6 = ghpcm(sx2, G=1:3, start= 0)
summary(ax6)
ax6

### plot results
plot(sx2,col = ax6$map + 1)

### use deterministic annealing for starting values
axDA = ghpcm(sx2, G=1:3, start=0,da=c(0.3,0.5,0.8,1.0))
summary(axDA)
axDA

## End(Not run)
```

gpcm

Gaussian Parsimonious Clustering Models

#### **Description**

Carries out model-based clustering or classification using some or all of the 14 parsimonious Gaussian clustering models (GPCM).

## Usage

```
gpcm(data=NULL, G=1:3, mnames=NULL,
start=2, label=NULL,
veo=FALSE, da=c(1.0),
nmax=1000, atol=1e-8, mtol=1e-8, mmax=10, burn=5,
pprogress=FALSE, pwarning=TRUE, stochastic = FALSE, seed=123)
```

#### **Arguments**

data A matrix or data frame such that rows correspond to observations and columns

correspond to variables. Note that this function currently only works with mul-

tivariate data p > 1.

G A sequence of integers giving the number of components to be used.

mnames The models (i.e., covariance structures) to be used. If NULL then all 14 are fitted.

start If 0 then the random soft function is used for initialization. If 1 then the random

hard function is used for initialization. If 2 then the kmeans function is used for initialization. If >2 then multiple random soft starts are used for initialization. If is.matrix then matrix is used as an initialization matrix as along as it has non-negative elements. Note: only models with the same number of columns of

this matrix will be fit.

label If NULL then the data has no known groups. If is.integer then some of the

observations have known groups. If label[i]=k then observation belongs to group k. If label[i]=0 then observation has no known group. See Examples.

veo Stands for "Variables exceed observations". If TRUE then if the number variables

in the model exceeds the number of observations the model is still fitted.

da Stands for Determinstic Annealing. A vector of doubles.

nmax The maximum number of iterations each EM algorithm is allowed to use.

atol A number specifying the epsilon value for the convergence criteria used in the

EM algorithms. For each algorithm, the criterion is based on the difference between the log-likelihood at an iteration and an asymptotic estimate of the loglikelihood at that iteration. This asymptotic estimate is based on the Aitken

acceleration and details are given in the References.

mtol A number specifying the epsilon value for the convergence criteria used in the

M-step in the GEM algorithms.

mmax The maximum number of iterations each M-step is allowed in the GEM algo-

rithms.

burn The burn in period for imputing data. (Missing observations are removed and a

model is estimated seperately before placing an imputation step within the EM.)

pprogress If TRUE print the progress of the function.

pwarning If TRUE print the warnings.

stochastic If TRUE, it will run stochastic E step variant.

seed The seed for the run, default is 123

#### **Details**

The data x are either clustered or classified using Gaussian mixture models with some or all of the 14 parsimonious covariance structures described in Celeux & Govaert (1995). The algorithms given by Celeux & Govaert (1995) is used for 12 of the 14 models; the "EVE" and "VVE" models use the algorithms given in Browne & McNicholas (2014). Starting values are very important to the successful operation of these algorithms and so care must be taken in the interpretation of results.

#### Value

An object of class gpcm is a list with components:

map A vector of integers indicating the maximum a posteriori classifications for the

best model.

model\_objs A list of all estimated models with parameters returned from the C++ call.

best\_model A class of gpcm\_best containing; the number of groups for the best model, the

covariance structure, and Bayesian Information Criterion (BIC) value.

loglik The log-likelihood values from fitting the best model.

z A matrix giving the raw values upon which map is based.

BIC A G by mnames by 3 dimensional array with values pertaining to BIC calcula-

tions. (legacy)

gpar A list object for each cluster pertaining to parameters. (legacy)

startobject The type of object inputted into start.

row\_tags If there were NAs in the original dataset, a vector of indices referencing the row

of the imputed vectors is given.

**Best Model:** An object of class gpcm\_best is a list with components:

model\_type A string containg summarized information about the type of model estimated

(Covariance structure and number of groups).

model\_obj An internal list containing all parameters returned from the C++ call.

BIC Bayesian Index Criterion (positive scale, bigger is better).

loglik Log liklihood from the estimated model.

nparam Number of a parameters in the mode.

startobject The type of object inputted into start.

G An integer representing the number of groups.

cov\_type A string representing the type of covariance matrix (see 14 models).

status Convergence status of EM algorithm according to Aitken's Acceleration

labs A vector of integers indicating the maximum a posteriori classifications for the

best model.

row\_tags If there were NAs in the original dataset, a vector of indices referencing the row

of the imputed vectors is given.

**Internal Objects:** All classes contain an internal list called model\_obj or model\_objs with the following components:

zigs	a posteori matrix
G	An integer representing the number of groups.
sigs	A vector of covariance matrices for each group
mus	A vector of mean vectors for each group

#### Note

Dedicated print, plot and summary functions are available for objects of class gpcm.

#### Author(s)

```
Nik Pocuca, Ryan P. Browne and Paul D. McNicholas.
```

Maintainer: Paul D. McNicholas <mcnicholas@math.mcmaster.ca>

#### References

McNicholas, P.D. (2016), *Mixture Model-Based Classification*. Boca Raton: Chapman & Hall/CRC Press

Browne, R.P. and McNicholas, P.D. (2014). Estimating common principal components in high dimensions. *Advances in Data Analysis and Classification* **8**(2), 217-226.

Celeux, G., Govaert, G. (1995). Gaussian parsimonious clustering models. *Pattern Recognition* **28**(5), 781-793.

```
## Not run:
data("x2")
### use kmeans to find starting values
ax0 = gpcm(x2, G=1:5, mnames=c("VVV", "EVE"), start=2, pprogress=TRUE, atol=1e-2)
summary(ax0)
ax0
### use random soft initializations.
ax6 = gpcm(x2, G=1:5, mnames=c("VVV", "EVE"),start= 0)
summary(ax6)
ax6
### use deterministic annealing for starting values
axDA = gpcm(x2, G=1:5, mnames=c("VVV", "EVE"), start=0, da=c(0.3, 0.5, 0.8, 1.0))
summary(axDA)
axDA
### estimate all 14 covariance structures
ax = gpcm(x2, G=1:5, mnames=NULL, start=0)
summary(ax)
### model based classification
x2.label = numeric(nrow(x2))
```

main\_loop 13

```
x2.label[c(10,50, 110, 150, 210, 250)] = c(1,1,2,2,3,3)
axl = gpcm(x2, G=3, mnames=c("VVV", "EVE"), label=x2.label)
summary(axl)

plot(x2, col = axl$map + 1)
## End(Not run)
```

main\_loop

GPCM Internal C++ Call

# **Description**

This function is the internal C++ function call within the gpcm function. This is a raw C++ function call, meaning it has no checks for proper inputs so it may fail to run without giving proper errors. Please ensure all arguements are valid. main\_loop is useful for writing parallizations of the gpcm function. All arguement descriptions are given in terms of their corresponding C++ types.

# Usage

# Arguments

X	A matrix or data frame such that rows correspond to observations and columns correspond to variables. Note that this function currently only works with multivariate data $p > 1$ .
G	A single positive integer value representing number of groups.
model_id	An integer representing the model_id, is useful for keeping track within parallizations. Not to be confused with model_type.
model_type	The type of covariance model you wish to run. Lexicon is given as follows: "0" = "EII", "1" = "VII", "2" = "EEI", "3" = "EVI", "4" = "VEI", "5" = "VVI", "6" = "EEE", "7" = "VEE", "8" = "EVE", "9" = "EEV", "10" = "VVE", "11" = "EVV", "12" = "VEV", "13" = "VVV"
in_zigs	A n times G a posteriori matrix resembling the probability of observation i belonging to group G. Rows must sum to one, have the proper dimensions, and be positive.
in_nmax	Positive integer value resembling the maximum amount of iterations for the EM.
in_l_tol	A likelihood tolerance for convergence.
in_m_iter_max	For certain models, where applicable, the number of iterations for the maximization step.
in_m_tol	For certain models, where applicable, the tolerance for the maximization step.

14 main\_loop

anneals A vector of doubles representing the deterministic annealing settings.

t\_burn A positive integer representing the number of burn steps if missing data (NAs)

are detected.

#### **Details**

Be extremly careful running this function, it is known to crash systems without proper exception handling. Consider using the package parallel to estimate all possible models at the same time.

#### Value

zigs	a postereori matrix
G	An integer representing the number of groups.
sigs	A vector of covariance matrices for each group (note you may have to reshape this)
mus	A vector of mean vectors for each group

#### Author(s)

Nik Pocuca, Ryan P. Browne and Paul D. McNicholas.

Maintainer: Paul D. McNicholas <mcnicholas@math.mcmaster.ca>

#### References

Browne, R.P. and McNicholas, P.D. (2014). Estimating common principal components in high dimensions. *Advances in Data Analysis and Classification* **8**(2), 217-226.

Zhou, H. and Lange, K. (2010). On the bumpy road to the dominant mode. *Scandinavian Journal of Statistics* **37**, 612-631.

Celeux, G., Govaert, G. (1995). Gaussian parsimonious clustering models. *Pattern Recognition* **28**(5), 781-793.

main\_loop\_gh

main\_loop\_gh

GHPCM Internal C++ Call

# **Description**

This function is the internal C++ function call within the ghpcm function. This is a raw C++ function call, meaning it has no checks for proper inputs so it may fail to run without giving proper errors. Please ensure all arguements are valid. main\_loop\_gh is useful for writing parallizations of the ghpcm function. All arguement descriptions are given in terms of their corresponding C++ types.

#### Usage

#### **Arguments**

Х	A matrix or data frame such that rows correspond to observations and columns correspond to variables. Note that this function currently only works with multivariate data $p > 1$ .
G	A single positive integer value representing number of groups.
model_id	An integer representing the model_id, is useful for keeping track within parallizations. Not to be confused with model_type.
model_type	The type of covariance model you wish to run. Lexicon is given as follows: "0" = "EII", "1" = "VII", "2" = "EEI", "3" = "EVI", "4" = "VEI", "5" = "VVI", "6" = "EEE", "7" = "VEE", "8" = "EVE", "9" = "EEV", "10" = "VVE", "11" = "EVV", "12" = "VEV", "13" = "VVV"
in_zigs	An times G a posteriori matrix resembling the probability of observation i be-

A n times G a posteriori matrix resembling the probability of observation i belonging to group G. Rows must sum to one, have the proper dimensions, and be positive.

main\_loop\_gh

in_nmax	Positive integer value resembling the maximum amount of iterations for the EM.
in_l_tol	A likelihood tolerance for convergence.
in_m_iter_max	For certain models, where applicable, the number of iterations for the maximization step.
in_m_tol	For certain models, where applicable, the tolerance for the maximization step.
anneals	A vector of doubles representing the deterministic annealing settings.
t_burn	A positive integer representing the number of burn steps if missing data (NAs) are detected.

#### **Details**

Be extremly careful running this function, it is known to crash systems without proper exception handling. Consider using the package parallel to estimate all possible models at the same time. Or run several possible initializations with random seeds.

#### Value

zigs	a postereori matrix
G	An integer representing the number of groups.
sigs	A vector of covariance matrices for each group (note you may have to reshape this)
mus	A vector of locational vectors for each group
alphas	A vector of skewness vectors for each group
omegas	First set of gamma parameters for each group
lambdas	Second set of gamma parameters for each group

#### Author(s)

Nik Pocuca, Ryan P. Browne and Paul D. McNicholas.

Maintainer: Paul D. McNicholas <mcnicholas@math.mcmaster.ca>

#### References

McNicholas, P.D. (2016), *Mixture Model-Based Classification*. Boca Raton: Chapman & Hall/CRC Press

Browne, R.P. and McNicholas, P.D. (2014). Estimating common principal components in high dimensions. *Advances in Data Analysis and Classification* **8**(2), 217-226.

Browne, R.P. and McNicholas, P.D. (2015), 'A mixture of generalized hyperbolic distributions', Canadian Journal of Statistics 43(2), 176-198.

Zhou, H. and Lange, K. (2010). On the bumpy road to the dominant mode. *Scandinavian Journal of Statistics* **37**, 612-631.

Celeux, G., Govaert, G. (1995). Gaussian parsimonious clustering models. *Pattern Recognition* **28**(5), 781-793.

main\_loop\_st 17

#### **Examples**

```
## Not run:
data("sx2")
data_in = as.matrix(sx2,ncol = 2)
n_{iter} = 300
in_g = 2
n = dim(data_in)[1]
model_string <- "VVV"</pre>
in_model_type <- switch(model_string, "EII" = 0,"VII" = 1,</pre>
               "EEI" = 2, "EVI" = 3, "VEI" = 4, "VVI" = 5, 
"VEE" = 7, "EVE" = 8, "EEV" = 9, "VVE" = 10,
                                                                    "EEE" = 6,
               "EVV" = 11, "VEV" = 12, "VVV" = 13)
zigs_in <- z_ig_random_soft(n,in_g)</pre>
m2 = main_loop_gh(X = t(data_in), # data in has to be in column major form
                G = 2, # number of groups
                model_id = 1, # model id for parallelization later
                model_type = in_model_type,
                in_zigs = zigs_in, # initializaiton
                in_nmax = n_iter, # number of iterations
                in_l_tol = 1e-8, # likilihood tolerance
                in_m_iter_max = 20, # maximium iterations for matrices
                in_m_tol = 1e-8,
                anneals=c(0.5,0.7,0.9,1)
plot(sx2,col = MAP(m2$zigs) + 1, cex = 0.5, pch = 20)
## End(Not run)
```

main\_loop\_st

STPCM Internal C++ Call

## Description

This function is the internal C++ function call within the stpcm function. This is a raw C++ function call, meaning it has no checks for proper inputs so it may fail to run without giving proper errors. Please ensure all arguements are valid. main\_loop\_st is useful for writing parallizations of the stpcm function. All arguement descriptions are given in terms of their corresponding C++ types.

# Usage

main\_loop\_st

# Arguments

X	A matrix or data frame such that rows correspond to observations and columns correspond to variables. Note that this function currently only works with multivariate data $p>1$ .
G	A single positive integer value representing number of groups.
model_id	An integer representing the model_id, is useful for keeping track within parallizations. Not to be confused with model_type.
model_type	The type of covariance model you wish to run. Lexicon is given as follows: "0" = "EII", "1" = "VII", "2" = "EEI", "3" = "EVI", "4" = "VEI", "5" = "VVI", "6" = "EEE", "7" = "VEE", "8" = "EVE", "9" = "EEV", "10" = "VVE", "11" = "EVV", "12" = "VEV", "13" = "VVV"
in_zigs	A n times G a posteriori matrix resembling the probability of observation i belonging to group G. Rows must sum to one, have the proper dimensions, and be positive.
in_nmax	Positive integer value resembling the maximum amount of iterations for the EM.
in_l_tol	A likelihood tolerance for convergence.
in_m_iter_max	For certain models, where applicable, the number of iterations for the maximization step.
in_m_tol	For certain models, where applicable, the tolerance for the maximization step.
anneals	A vector of doubles representing the deterministic annealing settings.
t_burn	A positive integer representing the number of burn steps if missing data (NAs) are detected.
latent_step	If "standard", it will use the standard E step for latent variable of a Normal Variance Mean Mixture, if "random" it will run a random draw from a GIG distribution.

# **Details**

Be extremly careful running this function, it is known to crash systems without proper exception handling. Consider using the package parallel to estimate all possible models at the same time. Or run several possible initializations with random seeds.

# Value

zigs	a postereori matrix
G	An integer representing the number of groups.
sigs	A vector of covariance matrices for each group (note you may have to reshape this)
mus	A vector of locational vectors for each group
alphas	A vector of skewness vectors for each group
vgs	Gamma parameters for each group

main\_loop\_st

#### Author(s)

Nik Pocuca, Ryan P. Browne and Paul D. McNicholas.

Maintainer: Paul D. McNicholas <mcnicholas@math.mcmaster.ca>

#### References

McNicholas, P.D. (2016), *Mixture Model-Based Classification*. Boca Raton: Chapman & Hall/CRC Press

Browne, R.P. and McNicholas, P.D. (2014). Estimating common principal components in high dimensions. *Advances in Data Analysis and Classification* **8**(2), 217-226.

Wei, Y., Tang, Y. and McNicholas, P.D. (2019), 'Mixtures of generalized hyperbolic distributions and mixtures of skew-t distributions for model-based clustering with incomplete data', Computational Statistics and Data Analysis 130, 18-41.

Zhou, H. and Lange, K. (2010). On the bumpy road to the dominant mode. *Scandinavian Journal of Statistics* **37**, 612-631.

Celeux, G., Govaert, G. (1995). Gaussian parsimonious clustering models. *Pattern Recognition* **28**(5), 781-793.

```
## Not run:
data("sx2")
data_in = as.matrix(sx2,ncol = 2)
n_{iter} = 300
in_g = 2
n = dim(data_in)[1]
model_string <- "VEI"</pre>
in_model_type <- switch(model_string, "EII" = 0,"VII" = 1,</pre>
              "EEI" = 2, "EVI" = 3, "VEI" = 4, "VVI" = 5, "EEE" = 6,
              "VEE" = 7, "EVE" = 8, "EEV" = 9, "VVE" = 10,
              "EVV" = 11, "VEV" = 12, "VVV" = 13)
zigs_in <- z_ig_random_soft(n,in_g)</pre>
m2 = main_loop_st(X = t(data_in), # data in has to be in column major form
               G = 2, # number of groups
               model_id = 1, # model id for parallelization later
               model_type = in_model_type,
               in_zigs = zigs_in, # initializaiton
               in_nmax = n_iter, # number of iterations
               in_l_tol = 0.5, # likilihood tolerance
               in_m_iter_max = 20, # maximium iterations for matrices
               anneals=c(1),
               in_m_tol = 1e-8
plot(sx2,col = MAP(m2$zigs) + 1, cex = 0.5, pch = 20)
## End(Not run)
```

20 main\_loop\_t

main_loop_t	TPCM Internal C++ Call	

# Description

This function is the internal C++ function call within the stpcm function. This is a raw C++ function call, meaning it has no checks for proper inputs so it may fail to run without giving proper errors. Please ensure all arguements are valid. main\_loop\_st is useful for writing parallizations of the stpcm function. All arguement descriptions are given in terms of their corresponding C++ types.

## Usage

# **Arguments**

X	A matrix or data frame such that rows correspond to observations and columns correspond to variables. Note that this function currently only works with multivariate data $p > 1$ .
G	A single positive integer value representing number of groups.
model_id	An integer representing the model_id, is useful for keeping track within parallizations. Not to be confused with model_type.
model_type	The type of covariance model you wish to run. Lexicon is given as follows: "0" = "EII", "1" = "VII", "2" = "EEI", "3" = "EVI", "4" = "VEI", "5" = "VVI", "6" = "EEE", "7" = "VEE", "8" = "EVE", "9" = "EEV", "10" = "VVE", "11" = "EVV", "12" = "VEV", "13" = "VVV"
in_zigs	A n times G a posteriori matrix resembling the probability of observation i belonging to group G. Rows must sum to one, have the proper dimensions, and be positive.
in_nmax	Positive integer value resembling the maximum amount of iterations for the EM.
in_l_tol	A likelihood tolerance for convergence.
in_m_iter_max	For certain models, where applicable, the number of iterations for the maximization step.
in_m_tol	For certain models, where applicable, the tolerance for the maximization step.
anneals	A vector of doubles representing the deterministic annealing settings.
t_burn	A positive integer representing the number of burn steps if missing data (NAs) are detected.

## **Details**

Be extremly careful running this function, it is known to crash systems without proper exception handling. Consider using the package parallel to estimate all possible models at the same time. Or run several possible initializations with random seeds.

main\_loop\_t 21

#### Value

zigs	a postereori matrix
G	An integer representing the number of groups.
sigs	A vector of covariance matrices for each group (note you may have to reshape this)
mus	A vector of locational vectors for each group
vgs	Gamma parameters for each group

#### Author(s)

Nik Pocuca, Ryan P. Browne and Paul D. McNicholas.

Maintainer: Paul D. McNicholas <mcnicholas@math.mcmaster.ca>

#### References

McNicholas, P.D. (2016), *Mixture Model-Based Classification*. Boca Raton: Chapman & Hall/CRC Press

Browne, R.P. and McNicholas, P.D. (2014). Estimating common principal components in high dimensions. *Advances in Data Analysis and Classification* **8**(2), 217-226.

Celeux, G., Govaert, G. (1995). Gaussian parsimonious clustering models. *Pattern Recognition* **28**(5), 781-793.

Andrews, J.L. and McNicholas, P.D. (2012), 'Model-based clustering, classification, and discriminant analysis via mixtures of multivariate t-distributions', Statistics and Computing 22(5), 1021-1029.

```
## Not run:
data("x2")
data_in = as.matrix(x2,ncol = 2)
n_{iter} = 300
in_g = 3
n = dim(data_in)[1]
model_string <- "VEI"</pre>
in_model_type <- switch(model_string, "EII" = 0,"VII" = 1,</pre>
               "EEI" = 2, "EVI" = 3, "VEI" = 4, "VVI" = 5, 
"VEE" = 7, "EVE" = 8, "EEV" = 9, "VVE" = 10,
                "EVV" = 11, "VEV" = 12, "VVV" = 13)
zigs_in <- z_ig_random_soft(n,in_g)</pre>
m2 = main_loop_t(X = data_in,
                 G = 3, # number of groups
                 model_id = 1, # model id for parallelization later
                 model_type = in_model_type,
                 in_zigs = zigs_in, # initializaiton
```

22 main\_loop\_vg

```
in_nmax = n_iter, # number of iterations
in_l_tol = 0.5, # likilihood tolerance
in_m_iter_max = 20, # maximium iterations for matrices
anneals=c(1),
in_m_tol = 1e-8)

plot(x2,col = MAP(m2$zigs) + 1, cex = 0.5, pch = 20)

## End(Not run)
```

main\_loop\_vg

VGPCM Internal C++ Call

# **Description**

This function is the internal C++ function call within the vgpcm function. This is a raw C++ function call, meaning it has no checks for proper inputs so it may fail to run without giving proper errors. Please ensure all arguements are valid. main\_loop\_vg is useful for writing parallizations of the stpcm function. All arguement descriptions are given in terms of their corresponding C++ types.

# Usage

# **Arguments**

X	A matrix or data frame such that rows correspond to observations and columns correspond to variables. Note that this function currently only works with multivariate data $p > 1$ .
G	A single positive integer value representing number of groups.
model_id	An integer representing the model_id, is useful for keeping track within parallizations. Not to be confused with model_type.
model_type	The type of covariance model you wish to run. Lexicon is given as follows: "0" = "EII", "1" = "VII", "2" = "EEI", "3" = "EVI", "4" = "VEI", "5" = "VVI", "6" = "EEE", "7" = "VEE", "8" = "EVE", "9" = "EEV", "10" = "VVE", "11" = "EVV", "12" = "VEV", "13" = "VVV"
in_zigs	A n times G a posteriori matrix resembling the probability of observation i belonging to group G. Rows must sum to one, have the proper dimensions, and be positive.
in_nmax	Positive integer value resembling the maximum amount of iterations for the EM.
in_l_tol	A likelihood tolerance for convergence.

main\_loop\_vg 23

in\_m\_iter\_max For certain models, where applicable, the number of iterations for the maximiza-

tion step.

in\_m\_tol For certain models, where applicable, the tolerance for the maximization step.

anneals A vector of doubles representing the deterministic annealing settings.

t\_burn A positive integer representing the number of burn steps if missing data (NAs)

are detected.

latent\_step If "standard", it will use the standard E step for latent variable of a Normal

Variance Mean Mixture, if "random" it will run a random draw from a GIG

distribution.

#### **Details**

Be extremly careful running this function, it is known to crash systems without proper exception handling. Consider using the package parallel to estimate all possible models at the same time. Or run several possible initializations with random seeds.

#### Value

zigs a postereori matrix

G An integer representing the number of groups.

sigs A vector of covariance matrices for each group (note you may have to reshape

this)

mus A vector of locational vectors for each group
alphas A vector of skewness vectors for each group

gammas Gamma parameters for each group

#### Author(s)

Nik Pocuca, Ryan P. Browne and Paul D. McNicholas.

Maintainer: Paul D. McNicholas <mcnicholas@math.mcmaster.ca>

#### References

McNicholas, P.D. (2016), *Mixture Model-Based Classification*. Boca Raton: Chapman & Hall/CRC Press

Browne, R.P. and McNicholas, P.D. (2014). Estimating common principal components in high dimensions. *Advances in Data Analysis and Classification* **8**(2), 217-226.

Zhou, H. and Lange, K. (2010). On the bumpy road to the dominant mode. *Scandinavian Journal of Statistics* **37**, 612-631.

Celeux, G., Govaert, G. (1995). Gaussian parsimonious clustering models. *Pattern Recognition* **28**(5), 781-793.

24 *MAP* 

#### **Examples**

```
## Not run:
data("sx2")
data_in = as.matrix(sx2,ncol = 2)
n_{iter} = 300
in_g = 2
n = dim(data_in)[1]
model_string <- "VVV"</pre>
in_model_type <- switch(model_string, "EII" = 0,"VII" = 1,
               "EEI" = 2, "EVI" = 3, "VEI" = 4, "VVI" = 5, 
"VEE" = 7, "EVE" = 8, "EEV" = 9, "VVE" = 10,
               "EVV" = 11, "VEV" = 12, "VVV" = 13)
zigs_in <- z_ig_random_soft(n,in_g)</pre>
m2 = main_loop_vg(X = t(data_in), # data in has to be in column major form
                G = 2, # number of groups
                model_id = 1, # model id for parallelization later
                model_type = in_model_type,
                in_zigs = zigs_in, # initializaiton
                in_nmax = n_iter, # number of iterations
                in_l_tol = 0.5, # likilihood tolerance
                in_m_iter_max = 20, # maximium iterations for matrices
                anneals=c(1),
                in_m_tol = 1e-8
plot(sx2, col = MAP(m2\$zigs) + 1, cex = 0.5, pch = 20)
## End(Not run)
```

MAP

Maximum a posterori

#### **Description**

Generates labels from a classification matrix z

## Usage

MAP(z\_ig)

# Arguments

z\_ig

A classification matrix of positive numbers in which all rows must sum to one.

# Value

A numeric matrix is returned of size n times g, with row sums adding up to 1.

mixture 25

#### Author(s)

Nik Pocuca, Ryan P. Browne and Paul D. McNicholas.

Maintainer: Paul D. McNicholas <mcnicholas@math.mcmaster.ca>

#### **Examples**

mixture

Mixture Models for Clustering and Classification

## Description

An implementation of 14 parsimonious clustering models for finite mixtures with components that are Gaussian, generalized hyperbolic, variance-gamma, Student's t, or skew-t, for model-based clustering and model-based classification, even with missing data.

## **Details**

Package: mixture
Type: Package
Version: 2.1.1
Date: 2024-01-29
License: GPL (>=2)

This package contains the functions gpcm, tpcm, ghpcm, vgpcm, stpcm, e\_step, ARI, and get\_best\_model, plus three simulated data sets.

This package also contains advanced functions for large system use which are: main\_loop\_wg , main\_loop\_gh, main\_loop\_t, main\_loop\_st, z\_ig\_random\_soft, z\_ig\_random\_hard, z\_ig\_kmeans.

26 pcm

#### Author(s)

Nik Pocuca, Ryan P. Browne, and Paul D. McNicholas.

Maintainer: Paul D. McNicholas <mcnicholas@math.mcmaster.ca>

#### See Also

Details, examples, and references are given under gpcm, tpcm, ghpcm, stpcm, and vgpcm.

pcm

Parsimonious Clustering Models

# Description

Carries out model-based clustering or classification using some or all of the 14 parsimonious settings with any one of the GPCM, VGPCM, or GHPCM families.

# Usage

```
pcm(data=NULL, G=1:3, pcmfamily=c(gpcm,vgpcm,tpcm),
mnames=NULL, start=2, label=NULL,
veo=FALSE, da=c(1.0),
nmax=1000, atol=1e-8, mtol=1e-8, mmax=10, burn=5,
pprogress=FALSE, pwarning=FALSE, seed=123)
```

# **Arguments**

data	A matrix or data frame such that rows correspond to observations and columns correspond to variables. Note that this function currently only works with multivariate data $p > 1$ .
G	A sequence of integers giving the number of components to be used.
pcmfamily	The family of models to be used. If NULL then all are fitted.
mnames	The models (i.e., covariance structures) to be used. If NULL then all 14 are fitted.
start	If 0 then the random soft function is used for initialization. If 1 then the random hard function is used for initialization. If 2 then the kmeans function is used for initialization. If >2 then multiple random soft starts are used for initialization. If is.matrix then matrix is used as an initialization matrix as along as it has non-negative elements. Note: only models with the same number of columns of this matrix will be fit.
label	If NULL then the data has no known groups. If is.integer then some of the observations have known groups. If label[i]=k then observation belongs to group k. If label[i]=0 then observation has no known group. See Examples.
veo	Stands for "Variables exceed observations". If TRUE then if the number variables in the model exceeds the number of observations the model is still fitted.
da	Stands for Determinstic Annealing. A vector of doubles.

pcm 27

nmax The maximum number of iterations each EM algorithm is allowed to use.

atol A number specifying the epsilon value for the convergence criteria used in the

EM algorithms. For each algorithm, the criterion is based on the difference between the log-likelihood at an iteration and an asymptotic estimate of the loglikelihood at that iteration. This asymptotic estimate is based on the Aitken

acceleration and details are given in the References.

mtol A number specifying the epsilon value for the convergence criteria used in the

M-step in the EM algorithms.

mmax The maximum number of iterations each M-step is allowed in the GEM algo-

rithms.

burn The burn in period for imputing data. (Missing observations are removed and a

model is estimated seperately before placing an imputation step within the EM.)

pprogress If TRUE print the progress of the function.

pwarning If TRUE print the warnings.

seed The seed for the run, default is 123

#### **Details**

The data x are either clustered or classified using Skew-t mixture models with some or all of the 14 parsimonious covariance structures described in Celeux & Govaert (1995). The algorithms given by Celeux & Govaert (1995) is used for 12 of the 14 models; the "EVE" and "VVE" models use the algorithms given in Browne & McNicholas (2014). Starting values are very important to the successful operation of these algorithms and so care must be taken in the interpretation of results.

#### Value

An object of class pcm is a list with components:

gpcm If applicable, the output of running the Gaussian Parsimonious Family.

vgpcm If applicable, the output of running the Variance-Gamma Parsimonious Family.

stpcm If applicable, the output of running the Skew-T Parsimonious Family.

ghpcm If applicable, the output of running the Generalized Hyperbolic Parsimonious

Family.

best\_model An object of corresponding to the output of the best performing family.

## Note

Dedicated print, and summary functions are available for objects of class pcm, gpcm, ghpcm, stpcm, or vgpcm.

#### Author(s)

Nik Pocuca, Ryan P. Browne and Paul D. McNicholas.

Maintainer: Paul D. McNicholas <mcnicholas@math.mcmaster.ca>

#### References

McNicholas, P.D. (2016), *Mixture Model-Based Classification*. Boca Raton: Chapman & Hall/CRC Press

Browne, R.P. and McNicholas, P.D. (2014). Estimating common principal components in high dimensions. *Advances in Data Analysis and Classification* **8**(2), 217-226.

Browne, R.P. and McNicholas, P.D. (2015), 'A mixture of generalized hyperbolic distributions', Canadian Journal of Statistics 43(2), 176-198.

Wei, Y., Tang, Y. and McNicholas, P.D. (2019), 'Mixtures of generalized hyperbolic distributions and mixtures of skew-t distributions for model-based clustering with incomplete data', Computational Statistics and Data Analysis 130, 18-41.

Celeux, G., Govaert, G. (1995). Gaussian parsimonious clustering models. *Pattern Recognition* **28**(5), 781-793.

# **Examples**

```
data("x2")
## Not run:
### estimate "VVV" "EVE"
ax = pcm(sx3, G=1:3, mnames=c("VVV", "EVE"), start=0)
summary(ax)
print(ax)
## End(Not run)
```

stpcm

Skew-t Parsimonious Clustering Models

# **Description**

Carries out model-based clustering or classification using some or all of the 14 parsimonious Skew-t clustering models (STPCM).

# Usage

```
stpcm(data=NULL, G=1:3, mnames=NULL,
start=2, label=NULL,
veo=FALSE, da=c(1.0),
nmax=1000, atol=1e-8, mtol=1e-8, mmax=10, burn=5,
pprogress=FALSE, pwarning=FALSE,
stochastic = FALSE, latent_method="standard", seed=123)
```

#### **Arguments**

data A matrix or data frame such that rows correspond to observations and columns

correspond to variables. Note that this function currently only works with mul-

tivariate data p > 1.

G A sequence of integers giving the number of components to be used.

mnames The models (i.e., covariance structures) to be used. If NULL then all 14 are fitted.

start If 0 then the random soft function is used for initialization. If 1 then the random

hard function is used for initialization. If 2 then the kmeans function is used for initialization. If >2 then multiple random soft starts are used for initialization. If is.matrix then matrix is used as an initialization matrix as along as it has non-negative elements. Note: only models with the same number of columns of

this matrix will be fit.

label If NULL then the data has no known groups. If is integer then some of the

observations have known groups. If label[i]=k then observation belongs to group k. If label[i]=0 then observation has no known group. See Examples.

veo Stands for "Variables exceed observations". If TRUE then if the number variables

in the model exceeds the number of observations the model is still fitted.

da Stands for Determinstic Annealing. A vector of doubles.

nmax The maximum number of iterations each EM algorithm is allowed to use.

atol A number specifying the epsilon value for the convergence criteria used in the

EM algorithms. For each algorithm, the criterion is based on the difference between the log-likelihood at an iteration and an asymptotic estimate of the loglikelihood at that iteration. This asymptotic estimate is based on the Aitken

acceleration and details are given in the References.

mtol A number specifying the epsilon value for the convergence criteria used in the

M-step in the EM algorithms.

mmax The maximum number of iterations each M-step is allowed in the GEM algo-

rithms.

burn The burn in period for imputing data. (Missing observations are removed and a

model is estimated seperately before placing an imputation step within the EM.)

pprogress If TRUE print the progress of the function.

pwarning If TRUE print the warnings.

stochastic If TRUE, it will run stochastic E step variant.

latent\_method If "standard", it will use the standard E step for latent variable of a Normal

Variance Mean Mixture, if "random" it will run a random draw from a GIG

distribution.

seed The seed for the run, default is 123

#### **Details**

The data x are either clustered or classified using Skew-t mixture models with some or all of the 14 parsimonious covariance structures described in Celeux & Govaert (1995). The algorithms given by Celeux & Govaert (1995) is used for 12 of the 14 models; the "EVE" and "VVE" models use the algorithms given in Browne & McNicholas (2014). Starting values are very important to the successful operation of these algorithms and so care must be taken in the interpretation of results.

#### Value

An object of class vgpcm is a list with components:

map A vector of integers indicating the maximum a posteriori classifications for the

best model.

model\_objs A list of all estimated models with parameters returned from the C++ call.

best\_model A class of vgpcm\_best containing; the number of groups for the best model, the

covariance structure, and Bayesian Information Criterion (BIC) value.

loglik The log-likelihood values from fitting the best model.

z A matrix giving the raw values upon which map is based.

BIC A G by mnames by 3 dimensional array with values pertaining to BIC calcula-

tions. (legacy)

gpar A list object for each cluster pertaining to parameters. (legacy)

startobject The type of object inputted into start.

row\_tags If there were NAs in the original dataset, a vector of indices referencing the row

of the imputed vectors is given.

**Best Model:** An object of class stpcm\_best is a list with components:

model\_type A string containg summarized information about the type of model estimated

(Covariance structure and number of groups).

model\_obj An internal list containing all parameters returned from the C++ call.

BIC Bayesian Index Criterion (positive scale, bigger is better).

loglik Log liklihood from the estimated model.

nparam Number of a parameters in the mode.

startobject The type of object inputted into start.

G An integer representing the number of groups.

cov\_type A string representing the type of covariance matrix (see 14 models).

Status Convergence status of EM algorithm according to Aitken's Acceleration

map A vector of integers indicating the maximum a posteriori classifications for the

best model.

row\_tags If there were NAs in the original dataset, a vector of indices referencing the row

of the imputed vectors is given.

**Internal Objects:** All classes contain an internal list called model\_obj or model\_objs with the following components:

zigs a posteori matrix

G An integer representing the number of groups.

sigs A vector of covariance matrices for each group

mus A vector of location vectors for each group

alphas A vector containg skewness vectors for each group

gammas A vector containing estimated gamma parameters for each group

#### Note

Dedicated print, plot and summary functions are available for objects of class vgpcm.

#### Author(s)

Nik Pocuca, Ryan P. Browne and Paul D. McNicholas.

Maintainer: Paul D. McNicholas <mcnicholas@math.mcmaster.ca>

#### References

McNicholas, P.D. (2016), *Mixture Model-Based Classification*. Boca Raton: Chapman & Hall/CRC Press

Browne, R.P. and McNicholas, P.D. (2014). Estimating common principal components in high dimensions. *Advances in Data Analysis and Classification* **8**(2), 217-226.

Wei, Y., Tang, Y. and McNicholas, P.D. (2019), 'Mixtures of generalized hyperbolic distributions and mixtures of skew-t distributions for model-based clustering with incomplete data', Computational Statistics and Data Analysis 130, 18-41.

Celeux, G., Govaert, G. (1995). Gaussian parsimonious clustering models. *Pattern Recognition* **28**(5), 781-793.

```
data("sx3")
## Not run:
### estimate "VVV" "EVE"
ax = stpcm(sx3, G=1:3, mnames=c("VVV","EVE"), start=0)
summary(ax)
ax

### estimate all 14 covariance structures
ax = stpcm(sx3, G=1:3, mnames=NULL, start=0)
summary(ax)
ax

### model based classification
sx3.label = c(rep(1,1000),rep(2,1000))
plot(sx3, col=sx3.label)
axl = stpcm(sx3, G=2, mnames=c("VVV", "EVE"), label=sx3.label)
summary(axl)

## End(Not run)
```

32 sx3

sx2

Skewed Simulated Data 1

# Description

Simulated data, with two variables and two groups, used to illustrate ghpcm, stpcm, vgpcm.

# Usage

```
data(sx2)
```

# **Format**

A data frame with 2000 observations and 2 columns.

#### **Source**

These data were simulated using R.

sx3

Skewed Simulated Data 2

# Description

Simulated data, with two variables and two groups, that are close together, used to illustrate ghpcm, stpcm, vgpcm.

# Usage

```
data(sx3)
```

# **Format**

A data frame with 2000 observations and 2 columns.

# Source

These data were simulated using R.

tpcm 33

tpcm

Student T Parsimonious Clustering Models

# Description

Carries out model-based clustering or classification using some or all of the 14 parsimonious Student T clustering models (TPCM).

# Usage

```
tpcm(data=NULL, G=1:3, mnames=NULL,
start=2, label=NULL,
veo=FALSE, da=c(1.0),
nmax=1000, atol=1e-8, mtol=1e-8, mmax=10, burn=5,
pprogress=FALSE, pwarning=FALSE, stochastic=FALSE,
constrained = FALSE, seed=123)
```

# Arguments

Suments	
data	A matrix or data frame such that rows correspond to observations and columns correspond to variables. Note that this function currently only works with multivariate data $p>1$ .
G	A sequence of integers giving the number of components to be used.
mnames	The models (i.e., covariance structures) to be used. If NULL then all 14 are fitted.
start	If 0 then the random soft function is used for initialization. If 1 then the random hard function is used for initialization. If 2 then the kmeans function is used for initialization. If >2 then multiple random soft starts are used for initialization. If is.matrix then matrix is used as an initialization matrix as along as it has non-negative elements. Note: only models with the same number of columns of this matrix will be fit.
label	If NULL then the data has no known groups. If is.integer then some of the observations have known groups. If label[i]=k then observation belongs to group k. If label[i]=0 then observation has no known group. See Examples.
veo	Stands for "Variables exceed observations". If TRUE then if the number variables in the model exceeds the number of observations the model is still fitted.
da	Stands for Determinstic Annealing. A vector of doubles.
nmax	The maximum number of iterations each EM algorithm is allowed to use.
atol	A number specifying the epsilon value for the convergence criteria used in the EM algorithms. For each algorithm, the criterion is based on the difference between the log-likelihood at an iteration and an asymptotic estimate of the log-likelihood at that iteration. This asymptotic estimate is based on the Aitken acceleration and details are given in the References.
mtol	A number specifying the epsilon value for the convergence criteria used in the M-step in the EM algorithms.

34 tpcm

mmax The maximum number of iterations each M-step is allowed in the GEM algo-

rithms.

burn The burn in period for imputing data. (Missing observations are removed and a

model is estimated seperately before placing an imputation step within the EM.)

pprogress If TRUE print the progress of the function.

pwarning If TRUE print the warnings.

stochastic If TRUE, it will run stochastic E step variant.

constrained If TRUE, it will constrain the degrees of freedom for student-t to be the same for

all clusters.

seed The seed for the run, default is 123

#### **Details**

The data x are either clustered or classified using Skew-t mixture models with some or all of the 14 parsimonious covariance structures described in Celeux & Govaert (1995). The algorithms given by Celeux & Govaert (1995) is used for 12 of the 14 models; the "EVE" and "VVE" models use the algorithms given in Browne & McNicholas (2014). Starting values are very important to the successful operation of these algorithms and so care must be taken in the interpretation of results.

#### Value

An object of class tpcm is a list with components:

map A vector of integers indicating the maximum a posteriori classifications for the

best model.

model\_objs A list of all estimated models with parameters returned from the C++ call.

best\_model A class of vgpcm\_best containing; the number of groups for the best model, the

covariance structure, and Bayesian Information Criterion (BIC) value.

loglik The log-likelihood values from fitting the best model.

z A matrix giving the raw values upon which map is based.

BIC A G by mnames by 3 dimensional array with values pertaining to BIC calcula-

tions. (legacy)

gpar A list object for each cluster pertaining to parameters. (legacy)

startobject The type of object inputted into start.

row\_tags If there were NAs in the original dataset, a vector of indices referencing the row

of the imputed vectors is given.

**Best Model:** An object of class stpcm\_best is a list with components:

model\_type A string containg summarized information about the type of model estimated

(Covariance structure and number of groups).

model\_obj An internal list containing all parameters returned from the C++ call.

BIC Bayesian Index Criterion (positive scale, bigger is better).

loglik Log liklihood from the estimated model.

tpcm 35

nparam Number of a parameters in the mode.
startobject The type of object inputted into start.

G An integer representing the number of groups.

cov\_type A string representing the type of covariance matrix (see 14 models).

status Convergence status of EM algorithm according to Aitken's Acceleration

map A vector of integers indicating the maximum a posteriori classifications for the

best model.

row\_tags If there were NAs in the original dataset, a vector of indices referencing the row

of the imputed vectors is given.

**Internal Objects:** All classes contain an internal list called model\_obj or model\_objs with the following components:

zigs a posteori matrix

G An integer representing the number of groups.

sigs A vector of covariance matrices for each group

mus A vector of location vectors for each group

vgs A vector containing estimated gamma parameters for each group

#### Note

Dedicated print, plot and summary functions are available for objects of class vgpcm.

#### Author(s)

Nik Pocuca, Ryan P. Browne and Paul D. McNicholas.

Maintainer: Paul D. McNicholas <mcnicholas@math.mcmaster.ca>

#### References

McNicholas, P.D. (2016), *Mixture Model-Based Classification*. Boca Raton: Chapman & Hall/CRC Press

Browne, R.P. and McNicholas, P.D. (2014). Estimating common principal components in high dimensions. *Advances in Data Analysis and Classification* **8**(2), 217-226.

Andrews, J.L. and McNicholas, P.D. (2012), 'Model-based clustering, classification, and discriminant analysis via mixtures of multivariate t-distributions', Statistics and Computing 22(5), 1021-1029.

Celeux, G., Govaert, G. (1995). Gaussian parsimonious clustering models. *Pattern Recognition* **28**(5), 781-793.

#### **Examples**

```
data("x2")
## Not run:
### estimate "VVV" "EVE"
ax = tpcm(x2, G=1:3, mnames=c("VVV", "EVE"), start=0)
summary(ax)
ax

### estimate all 14 covariance structures
ax = tpcm(x2, G=1:3, mnames=NULL, start=0)
summary(ax)
ax

## End(Not run)
```

vgpcm

Variance Gamma Parsimonious Clustering Models

# Description

Carries out model-based clustering or classification using some or all of the 14 parsimonious Variance Gamma clustering models (VGPCM).

# Usage

```
vgpcm(data=NULL, G=1:3, mnames=NULL,
start=2, label=NULL,
veo=FALSE, da=c(1.0),
nmax=1000, atol=1e-8, mtol=1e-8, mmax=10, burn=5,
pprogress=FALSE, pwarning=FALSE,
stochastic = FALSE, latent_method="standard", seed=123)
```

# **Arguments**

data	A matrix or data frame such that rows correspond to observations and columns correspond to variables. Note that this function currently only works with multivariate data $p > 1$ .
G	A sequence of integers giving the number of components to be used.
mnames	The models (i.e., covariance structures) to be used. If NULL then all 14 are fitted.
start	If 0 then the random soft function is used for initialization. If 1 then the random hard function is used for initialization. If 2 then the kmeans function is used for initialization. If >2 then multiple random soft starts are used for initialization.

If is.matrix then matrix is used as an initialization matrix as along as it has non-negative elements. Note: only models with the same number of columns of

this matrix will be fit.

label If NULL then the data has no known groups. If is.integer then some of the

observations have known groups. If label[i]=k then observation belongs to group k. If label[i]=0 then observation has no known group. See Examples.

veo Stands for "Variables exceed observations". If TRUE then if the number variables

in the model exceeds the number of observations the model is still fitted.

da Stands for Determinstic Annealing. A vector of doubles.

nmax The maximum number of iterations each EM algorithm is allowed to use.

atol A number specifying the epsilon value for the convergence criteria used in the

EM algorithms. For each algorithm, the criterion is based on the difference between the log-likelihood at an iteration and an asymptotic estimate of the loglikelihood at that iteration. This asymptotic estimate is based on the Aitken

acceleration and details are given in the References.

mtol A number specifying the epsilon value for the convergence criteria used in the

M-step in the EM algorithms.

mmax The maximum number of iterations each M-step is allowed in the GEM algo-

rithms.

burn The burn in period for imputing data. (Missing observations are removed and a

model is estimated seperately before placing an imputation step within the EM.)

pprogress If TRUE print the progress of the function.

pwarning If TRUE print the warnings.

stochastic If TRUE, it will run stochastic E step variant.

latent\_method If "standard", it will use the standard E step for latent variable of a Normal

Variance Mean Mixture, if "random" it will run a random draw from a GIG

distribution.

seed The seed for the run, default is 123

#### **Details**

The data x are either clustered or classified using Variance Gamma mixture models with some or all of the 14 parsimonious covariance structures described in Celeux & Govaert (1995). The algorithms given by Celeux & Govaert (1995) is used for 12 of the 14 models; the "EVE" and "VVE" models use the algorithms given in Browne & McNicholas (2014). Starting values are very important to the successful operation of these algorithms and so care must be taken in the interpretation of results.

## Value

An object of class vgpcm is a list with components:

map A vector of integers indicating the maximum a posteriori classifications for the

best model.

model\_objs A list of all estimated models with parameters returned from the C++ call.

best\_model A class of vgpcm\_best containing; the number of groups for the best model, the

covariance structure, and Bayesian Information Criterion (BIC) value.

loglik The log-likelihood values from fitting the best model.

z A matrix giving the raw values upon which map is based.

BIC A G by mnames by 3 dimensional array with values pertaining to BIC calcula-

tions. (legacy)

startobject The type of object inputted into start.

gpar A list object for each cluster pertaining to parameters. (legacy)

row\_tags If there were NAs in the original dataset, a vector of indices referencing the row

of the imputed vectors is given.

**Best Model:** An object of class vgpcm\_best is a list with components:

model\_type A string containg summarized information about the type of model estimated

(Covariance structure and number of groups).

model\_obj An internal list containing all parameters returned from the C++ call.

BIC Bayesian Index Criterion (positive scale, bigger is better).

loglik Log liklihood from the estimated model.

nparam Number of a parameters in the mode.

startobject The type of object inputted into start.

G An integer representing the number of groups.

cov\_type A string representing the type of covariance matrix (see 14 models).

Status Convergence status of EM algorithm according to Aitken's Acceleration

map A vector of integers indicating the maximum a posteriori classifications for the

best model.

row\_tags If there were NAs in the original dataset, a vector of indices referencing the row

of the imputed vectors is given.

**Internal Objects:** All classes contain an internal list called model\_obj or model\_objs with the following components:

zigs a posteori matrix

An integer representing the number of groups.

sigs A vector of covariance matrices for each group

mus A vector of location vectors for each group

alphas A vector containg skewness vectors for each group

gammas A vector containing estimated gamma parameters for each group

#### Note

Dedicated print, plot and summary functions are available for objects of class vgpcm.

#### Author(s)

Nik Pocuca, Ryan P. Browne and Paul D. McNicholas.

Maintainer: Paul D. McNicholas <mcnicholas@math.mcmaster.ca>

#### References

McNicholas, P.D. (2016), *Mixture Model-Based Classification*. Boca Raton: Chapman & Hall/CRC Press

Browne, R.P. and McNicholas, P.D. (2014). Estimating common principal components in high dimensions. *Advances in Data Analysis and Classification* **8**(2), 217-226.

Celeux, G., Govaert, G. (1995). Gaussian parsimonious clustering models. *Pattern Recognition* **28**(5), 781-793.

```
## Not run:
data("sx2")
### use kmeans to find starting values
ax0 = vgpcm(sx2, G=1:3, mnames=c("VVV", "EVE"), start=2, pprogress=TRUE, atol=1e-2)
summary(ax0)
ax0
### use random soft initializations.
ax6 = vgpcm(sx2, G=1:3, mnames=c("VVV", "EVE"),start= 0)
summary(ax6)
ax6
### use deterministic annealing for starting values
axDA = vgpcm(sx2, G=1:3, mnames=c("VVV", "EVE"), start=0,da=c(0.3,0.5,0.8,1.0))
summary(axDA)
axDA
### estimate all 14 covariance structures
ax = vgpcm(sx2, G=1:3, mnames=NULL, start=0)
summary(ax)
ax
### model based classification
sx2.label = c(rep(1,1000), rep(2,1000))
plot(sx2, col=sx2.label)
axl = vgpcm(sx2, G=2, mnames=c("VVV", "EVE"), label=sx2.label)
summary(axl)
## End(Not run)
```

z\_ig\_kmeans

x2

Simulated Data

### **Description**

Simulated data, with two variables with three groups, used to illustrate gpcm.

# Usage

```
data(x2)
```

#### **Format**

A data frame with 300 observations and 2 columns.

#### **Source**

These data were simulated using R.

z\_ig\_kmeans

K-means Initialization

# **Description**

Generates an initialization matrix for a dataset X using k-means.

# Usage

```
z_ig_kmeans(X,g)
```

# **Arguments**

X A matrix or data frame such that rows correspond to observations and columns

correspond to variables. Note that this function currently only works with mul-

tivariate data p > 1. Note. NO NAS allowed.

g An integer representing the number of groups.

## Value

A numeric matrix is returned of size n times g, with row sums adding up to 1.

# Author(s)

Nik Pocuca, Ryan P. Browne and Paul D. McNicholas.

Maintainer: Paul D. McNicholas <mcnicholas@math.mcmaster.ca>

z\_ig\_random\_hard 41

#### References

Browne, R.P. and McNicholas, P.D. (2014). Estimating common principal components in high dimensions. *Advances in Data Analysis and Classification* **8**(2), 217-226.

Zhou, H. and Lange, K. (2010). On the bumpy road to the dominant mode. *Scandinavian Journal of Statistics* **37**, 612-631.

Celeux, G., Govaert, G. (1995). Gaussian parsimonious clustering models. *Pattern Recognition* **28**(5), 781-793.

## **Examples**

```
#data("x2")
#z_init <- z_ig_kmeans(x2,g=3)</pre>
```

z\_ig\_random\_hard

Random Hard Initialization

## **Description**

Generates an initialization matrix of size n times g using random hard.

## Usage

```
z_ig_random_hard(n,g)
```

## **Arguments**

n Number of rows, must be positive.

g Number of columns, must be positive.

#### Author(s)

Nik Pocuca, Ryan P. Browne and Paul D. McNicholas.

Maintainer: Paul D. McNicholas <mcnicholas@math.mcmaster.ca>

# References

Browne, R.P. and McNicholas, P.D. (2014). Estimating common principal components in high dimensions. *Advances in Data Analysis and Classification* **8**(2), 217-226.

Zhou, H. and Lange, K. (2010). On the bumpy road to the dominant mode. *Scandinavian Journal of Statistics* **37**, 612-631.

Celeux, G., Govaert, G. (1995). Gaussian parsimonious clustering models. *Pattern Recognition* **28**(5), 781-793.

```
z_init <- z_ig_random_hard(100,3)</pre>
```

42 z\_ig\_random\_soft

z\_ig\_random\_soft

Random Soft Initialization

# **Description**

Generates an initialization matrix of size n times g using random soft.

# Usage

```
z_{ig}_{n,g}
```

# Arguments

n Number of rows, must be positive.

g Number of columns, must be positive.

## Author(s)

Nik Pocuca, Ryan P. Browne and Paul D. McNicholas.

Maintainer: Paul D. McNicholas <mcnicholas@math.mcmaster.ca>

# References

Browne, R.P. and McNicholas, P.D. (2014). Estimating common principal components in high dimensions. *Advances in Data Analysis and Classification* **8**(2), 217-226.

Zhou, H. and Lange, K. (2010). On the bumpy road to the dominant mode. *Scandinavian Journal of Statistics* **37**, 612-631.

Celeux, G., Govaert, G. (1995). Gaussian parsimonious clustering models. *Pattern Recognition* **28**(5), 781-793.

```
z_{init} \leftarrow z_{ig_random_soft(100,3)}
```

# **Index**

* classif	sx2, 32
ARI, 2	sx3, 32
e_step, 3	x2, 40
<pre>get_best_model, 5</pre>	* multivariate
ghpcm, 6	ARI, 2
gpcm, 9	e_step, 3
main_loop, 13	<pre>get_best_model, 5</pre>
main_loop_gh, 15	ghpcm, 6
main_loop_st, 17	gpcm, 9
main_loop_t, 20	main_loop, 13
main_loop_vg, 22	main_loop_gh, 15
MAP, 24	<pre>main_loop_st, 17</pre>
pcm, 26	main_loop_t, 20
stpcm, 28	main_loop_vg, 22
tpcm, 33	MAP, 24
vgpcm, 36	pcm, 26
z_ig_kmeans, 40	stpcm, 28
z_ig_random_hard,41	tpcm, 33
z_ig_random_soft,42	vgpcm, 36
* cluster	z_ig_kmeans, 40
ARI, 2	z_ig_random_hard, 41
e_step, 3	z_ig_random_soft,42
<pre>get_best_model, 5</pre>	ARI, 2
ghpcm, 6	ARI, Z
gpcm, 9	e_step, 3
main_loop, 13	_ '/
main_loop_gh, 15	<pre>get_best_model, 5</pre>
main_loop_st, 17	ghpcm, 6, 26, 32
main_loop_t, 20	gpcm, 9, 26, 40
main_loop_vg, 22	
MAP, 24	main_loop, 13
pcm, 26	main_loop_gh, 15
stpcm, 28	main_loop_st, 17
tpcm, 33	main_loop_t, 20
vgpcm, 36	main_loop_vg, 22
z_ig_kmeans, 40	MAP, 24
z_ig_random_hard, 41	mixture, 25
z_ig_random_soft, 42	mixture-package (mixture), 25
* datasets	pcm, 26
· www.sets	Poiii, 20

44 INDEX

```
stpcm, 26, 28, 32

sx2, 32

sx3, 32

tpcm, 26, 33

vgpcm, 26, 32, 36

x2, 40

z_ig_kmeans, 40

z_ig_random_hard, 41

z_ig_random_soft, 42
```