# Package 'NPflow'

January 13, 2024

| Type Package   |
|--|
| <b>Title</b> Bayesian Nonparametrics for Automatic Gating of Flow-Cytometry Data   |
| Version 0.13.5   |
| <b>Date</b> 2024-01-13   |
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| Suggests foreach, parallel, doParallel, itertools, microbenchmark  |
| <b>Description</b> Dirichlet process mixture of multivariate normal, skew normal or skew t-distributions modeling oriented towards flow-cytometry data preprocessing applications. Method is detailed in: Hejblum, Alkhassimn, Gottardo, Caron & Thiebaut (2019) <doi:10.1214 18-aoas1209="">.</doi:10.1214> |
| License LGPL-3   file LICENSE  |
| BugReports https://github.com/sistm/NPflow/issues  |
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| NPflow-package   |

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## **Description**

Dirichlet process mixture of multivariate normal, skew normal or skew t-distributions modeling oriented towards flow-cytometry data pre-processing applications.

## **Details**

Package: NPflow
Type: Package
Version: 0.13.5
Date: 2024-01-13
License: LGPL-3

The main function in this package is DPMpost.

## Author(s)

Boris P. Hejblum, Chariff Alkhassim, Francois Caron — Maintainer: Boris P. Hejblum

## References

Hejblum BP, Alkhassim C, Gottardo R, Caron F and Thiebaut R (2019) Sequential Dirichlet Process Mixtures of Multivariate Skew t-distributions for Model-based Clustering of Flow Cytometry Data. The Annals of Applied Statistics, 13(1): 638-660. <a href="https://arxiv.org/abs/1702.04407">doi:10.1214/18-AOAS1209</a> <a href="https://arxiv.org/abs/1702.04407">arXiv:org/abs/1702.04407</a> doi:10.1214/18AOAS1209

## See Also

Useful links:

• Report bugs at https://github.com/sistm/NPflow/issues

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burn.DPMMclust

Burning MCMC iterations from a Dirichlet Process Mixture Model.

## Description

Utility function for burning MCMC iteration from a DPMMclust object.

## Usage

```
burn.DPMMclust(x, burnin = 0, thin = 1)
```

## **Arguments**

x a DPMMclust object.

burnin the number of MCMC iterations to burn (default is  $\emptyset$ ).

thin the spacing at which MCMC iterations are kept. Default is 1, i.e. no thining.

#### Value

a DPMMclust object minus the burnt iterations

## Author(s)

Boris Hejblum

#### See Also

summary.DPMMclust

cluster\_est\_binder

Point estimate of the partition for the Binder loss function

## Description

Get a point estimate of the partition using the Binder loss function.

## Usage

```
cluster_est_binder(c, logposterior)
```

## **Arguments**

c a list of vector of length n. c[[j]][i] is the cluster allocation of observation

i=1...n at iteration j=1...N.

logposterior vector of logposterior corresponding to each partition from c used to break ties

when minimizing the cost function

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## Value

```
a list:
c_est: a vector of length n. Point estimate of the partition
cost: a vector of length N. cost[j] is the cost associated to partition c[[j]]
similarity: matrix of size n x n. Similarity matrix (see similarityMat)
opt_ind: the index of the optimal partition among the MCMC iterations.
```

## Author(s)

Francois Caron, Boris Hejblum

#### References

F Caron, YW Teh, TB Murphy, Bayesian nonparametric Plackett-Luce models for the analysis of preferences for college degree programmes, Annals of Applied Statistics, 8(2):1145-1181, 2014.

DB Dahl, Model-Based Clustering for Expression Data via a Dirichlet Process Mixture Model, Bayesian Inference for Gene Expression and Proteomics, K-A Do, P Muller, M Vannucci (Eds.), Cambridge University Press, 2006.

#### See Also

```
similarityMat similarityMatC
```

```
cluster_est_Fmeasure
                          Point estimate of the partition using the F-measure as the cost func-
```

## **Description**

Get a point estimate of the partition using the F-measure as the cost function.

## Usage

```
cluster_est_Fmeasure(c, logposterior)
```

## **Arguments**

С a list of vector of length n. c[[j]][i] is the cluster allocation of observation i=1...n at iteration j=1...N. logposterior a vector of logposterior corresponding to each partition from c used to break ties

when minimizing the cost function

## Value

a list:

c\_est: a vector of length n. Point estimate of the partition

cost: a vector of length N. cost[j] is the cost associated to partition c[[j]]

similarity: matrix of size n x n. Similarity matrix (see similarityMat) opt\_ind: the index of the optimal partition among the MCMC iterations.

## Author(s)

Francois Caron, Boris Hejblum

## See Also

similarityMat

cluster\_est\_Mbinder\_norm

Point estimate of the partition using a modified Binder loss function

## Description

Get a point estimate of the partition using a modified Binder loss function for Gaussian components

## Usage

```
cluster_est_Mbinder_norm(c, Mu, Sigma, lambda = 0, a = 1, b = a, logposterior)
```

## **Arguments**

| С | a list of vector of length n. c[[j]][i] is the cluster allocation of observation |
|---|--|
|   | i=1n at iteration j=1N.  |

Mu is a list of length n composed of p x 1 matrices. Where 1 is the maximum num-

ber of components per partition.

Sigma is list of length n composed of arrays containing a maximum of 1 p x p covari-

ance matrices.

lambda is a nonnegative tunning parameter allowing further control over the distance

function. Default is 0.

a nonnegative constant seen as the unit cost for pairwise misclassification. Default

is 1.

b nonnegative constant seen as the unit cost for the other kind of pairwise misclas-

sification. Default is 1.

logposterior vector of logposterior corresponding to each partition from c used to break ties

when minimizing the cost function

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## **Details**

Note that he current implementation only allows Gaussian components.

The modified Binder loss function takes into account the distance between mixture components using #'the Bhattacharyya distance.

## Value

a list:

c\_est: a vector of length n. Point estimate of the partition

cost: a vector of length N. cost[j] is the cost associated to partition c[[j]]

similarity: matrix of size n x n. Similarity matrix (see similarityMat) opt\_ind: the index of the optimal partition among the MCMC iterations.

## Author(s)

Chariff Alkhassim

#### References

JW Lau, PJ Green, Bayesian Model-Based Clustering Procedures, *Journal of Computational and Graphical Statistics*, 16(3):526-558, 2007.

DA Binder, Bayesian cluster analysis, Biometrika 65(1):31-38, 1978.

## See Also

```
similarityMat similarityMatC similarityMat_nocostC
```

| cluster_est_pear | Gets a point estimate of the partition using posterior expected adjusted |
|------------------|--|
|                  | Rand index (PEAR)  |

## Description

Gets a point estimate of the partition using posterior expected adjusted Rand index (PEAR)

## Usage

```
cluster_est_pear(c)
```

#### **Arguments**

```
c a list of vector of length n. c[[j]][i] is the cluster allocation of observation i=1...n at iteration j=1...N.
```

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## Value

a list:

c\_est: a vector of length n. Point estimate of the partition

pear: a vector of length N. pear[j] is the posterior expected adjusted Rand index

associated to partition c[[j]]

similarity: matrix of size n x n. Similarity matrix (see similarityMat)

opt\_ind: the index of the optimal partition among the MCMC iterations.

## Author(s)

Chariff Alkhassim

## References

A. Fritsch, K. Ickstadt. Improved Criteria for Clustering Based on the Posterior Similarity Matrix, in Bayesian Analysis, Vol.4: p.367-392 (2009)

## See Also

```
similarityMat similarityMatC
```

cytoScatter

Scatterplot of flow cytometry data

## **Description**

Scatterplot of flow cytometry data

# Usage

```
cytoScatter(
  cytomatrix,
  dims2plot = c(1, 2),
  gating = NULL,
  scale_log = FALSE,
  xlim = NULL,
  ylim = NULL,
  gg.add = list(theme())
)
```

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## **Arguments**

| cytomatrix | a p x n data matrix, of n cell observations measured over p markers.   |
|------------|--|
| dims2plot  | a vector of length at least 2, indicating of the dimensions to be plotted. Default is $c(1, 2)$ .  |
| gating     | an optional vector of length n indicating a known gating of the cells to be displayed. Default is NULL in which case no gating is displayed. |
| scale_log  | a logical Flag indicating whether the data should be plotted on the log scale. Default is FALSE.   |
| xlim       | a vector of length 2 to specify the x-axis limits. Only used if $dims2plot$ is of length 2Default is the data range.                         |
| ylim       | a vector of length 2 to specify the y-axis limits. Only used if $dims2plot$ is of length 2. Default is the data range.                       |
| gg.add     | A list of instructions to add to the ggplot2 instruction (see gg-add). Default is list(theme()), which adds nothing. to the plot.            |

```
rm(list=ls())
#Number of data
n <- 500
#n <- 2000
set.seed(1234)
#set.seed(123)
#set.seed(4321)
# Sample data
m <- matrix(nrow=2, ncol=4, c(-1, 1, 1.5, 2, 2, -2, -1.5, -2))
p \leftarrow c(0.2, 0.1, 0.4, 0.3) # frequence des clusters
sdev <- array(dim=c(2,2,4))</pre>
sdev[, ,1] \leftarrow matrix(nrow=2, ncol=2, c(0.3, 0, 0, 0.3))
sdev[, ,2] <- matrix(nrow=2, ncol=2, c(0.1, 0, 0, 0.3))</pre>
sdev[, ,3] \leftarrow matrix(nrow=2, ncol=2, c(0.3, 0.15, 0.15, 0.3))
sdev[, ,4] <- .3*diag(2)</pre>
c \leftarrow rep(0,n)
z <- matrix(0, nrow=2, ncol=n)</pre>
for(k in 1:n){
c[k] = which(rmultinom(n=1, size=1, prob=p)!=0)
z[,k] \leftarrow m[, c[k]] + sdev[, , c[k]]**matrix(rnorm(2, mean = 0, sd = 1), nrow=2, ncol=1)
 \#cat(k, "/", n, " observations simulated\n", sep="")
}
cytoScatter(z)
```

| DPMGibbsN | Slice Sampling of the Dirichlet Process Mixture Model with a prior on alpha |
|-----------|---|
|           |   |

# Description

Slice Sampling of the Dirichlet Process Mixture Model with a prior on alpha

# Usage

```
DPMGibbsN(
   z,
   hyperG0,
   a = 1e-04,
   b = 1e-04,
   N,
   doPlot = TRUE,
   nbclust_init = 30,
   plotevery = N/10,
   diagVar = TRUE,
   use_variance_hyperprior = TRUE,
   verbose = TRUE,
   ...
)
```

## Arguments

| Z            | data matrix d x n with d dimensions in rows and n observations in columns.  |
|--------------|---|
| hyperG0      | prior mixing distribution.  |
| a            | shape hyperparameter of the Gamma prior on the concentration parameter of the Dirichlet Process. Default is $0.0001$ .  |
| b            | scale hyperparameter of the Gamma prior on the concentration parameter of the Dirichlet Process. Default is 0.0001. If 0, then the concentration is fixed set to a. |
| N            | number of MCMC iterations.  |
| doPlot       | logical flag indicating whether to plot MCMC iteration or not. Default to TRUE.   |
| nbclust_init | number of clusters at initialization. Default to 30 (or less if there are less than 30 observations).   |
| plotevery    | an integer indicating the interval between plotted iterations when doPlot is $\ensuremath{TRUE}.$   |
| diagVar      | logical flag indicating whether the variance of each cluster is estimated as a diagonal matrix, or as a full matrix. Default is TRUE (diagonal variance).           |

use\_variance\_hyperprior

logical flag indicating whether a hyperprior is added for the variance parameter. Default is TRUE which decrease the impact of the variance prior on the posterior.

FALSE is useful for using an informative prior.

verbose logical flag indicating whether partition info is written in the console at each

MCMC iteration.

... additional arguments to be passed to plot\_DPM. Only used if doPlot is TRUE.

#### Value

a object of class DPMclust with the following attributes:

mcmc\_partitions:

a list of length N. Each element mcmc\_partitions[n] is a vector of length n

giving the partition of the n observations.

alpha: a vector of length N. cost[j] is the cost associated to partition c[[j]]

listU\_mu: a list of length N containing the matrices of mean vectors for all the mixture

components at each MCMC iteration

listU\_Sigma: a list of length N containing the arrays of covariances matrices for all the mixture

components at each MCMC iteration

U\_SS\_list: a list of length N containing the lists of sufficient statistics for all the mixture

components at each MCMC iteration

weights\_list: a list of length N containing the logposterior values at each MCMC iterations

logposterior\_list:

a list of length N containing the logposterior values at each MCMC iterations

data: the data matrix d x n with d dimensions in rows and n observations in columns.

nb\_mcmcit: the number of MCMC iterations

clust\_distrib: the parametric distribution of the mixture component - "gaussian"

hyperG0: the prior on the cluster location

#### Author(s)

Boris Hejblum

```
rm(list=ls())
#Number of data
n <- 500
d <- 4
#n <- 2000
set.seed(1234)
#set.seed(123)
#set.seed(4321)
# Sample data
m <- matrix(nrow=d, ncol=4, c(-1, 1, 1.5, 2, 2, -2, -1.5, -2))</pre>
```

```
p \leftarrow c(0.2, 0.1, 0.4, 0.3) # frequence des clusters
sdev <- array(dim=c(d,d,4))</pre>
sdev[, ,1] <- 0.3*diag(d)
sdev[, ,2] \leftarrow c(0.1, 0.3)*diag(d)
sdev[, ,3] <- matrix(nrow=d, ncol=d, 0.15)</pre>
diag(sdev[, ,3]) \leftarrow 0.3
sdev[, ,4] <- 0.3*diag(d)
c \leftarrow rep(0,n)
z <- matrix(0, nrow=d, ncol=n)</pre>
for(k in 1:n){
 c[k] = which(rmultinom(n=1, size=1, prob=p)!=0)
 z[,k] \leftarrow m[, c[k]] + sdev[, , c[k]]**matrix(rnorm(d, mean = 0, sd = 1), nrow=d, ncol=1)
 \#cat(k, "/", n, " observations simulated\n", sep="")
}
 # Set parameters of G0
 hyperG0 <- list()</pre>
 hyperG0[["mu"]] <- rep(0,d)
 hyperG0[["kappa"]] <- 0.001
 hyperG0[["nu"]] <- d+2
 hyperG0[["lambda"]] \leftarrow diag(d)/10
 # hyperprior on the Scale parameter of DPM
 a <- 0.0001
 b <- 0.0001
 # Number of iterations
 N <- 30
 # do some plots
 doPlot <- TRUE
 nbclust_init <- 30</pre>
 ## Data
 ########
 library(ggplot2)
 p \leftarrow (ggplot(data.frame("X"=z[1,], "Y"=z[2,]), aes(x=X, y=Y))
       + geom_point()
       + ggtitle("Toy example Data"))
 р
 ## alpha priors plots
 ########################
 prioralpha <- data.frame("alpha"=rgamma(n=5000, shape=a, scale=1/b),</pre>
                           "distribution" =factor(rep("prior",5000),
                           levels=c("prior", "posterior")))
 p <- (ggplot(prioralpha, aes(x=alpha))</pre>
       + geom_histogram(aes(y=..density..),
                          colour="black", fill="white", bins=30)
```

```
+ geom_density(alpha=.6, fill="red", color=NA)
      + ggtitle(paste("Prior distribution on alpha: Gamma(", a,
                ",", b, ")\n", sep=""))
      + theme_bw()
p
if(interactive()){
# Gibbs sampler for Dirichlet Process Mixtures
MCMCsample <- DPMGibbsN(z, hyperG0, a, b, N=500, doPlot, nbclust_init, plotevery=100,
                         gg.add=list(theme_bw(),
                        guides(shape=guide_legend(override.aes = list(fill="grey45")))),
                        diagVar=FALSE)
plot_ConvDPM(MCMCsample, from=2)
s <- summary(MCMCsample, burnin = 200, thin=2, posterior_approx=FALSE,</pre>
lossFn = "MBinderN")
F <- FmeasureC(pred=s$point_estim$c_est, ref=c)</pre>
postalpha <- data.frame("alpha"=MCMCsample$alpha[50:500],</pre>
                         "distribution" = factor(rep("posterior",500-49),
                        levels=c("prior", "posterior")))
p <- (ggplot(postalpha, aes(x=alpha))</pre>
      + geom_histogram(aes(y=..density..), binwidth=.1,
                       colour="black", fill="white")
      + geom_density(alpha=.2, fill="blue")
      + ggtitle("Posterior distribution of alpha\n")
      # Ignore NA values for mean
      # Overlay with transparent density plot
      + geom_vline(aes(xintercept=mean(alpha, na.rm=TRUE)),
                   color="red", linetype="dashed", size=1)
    )
р
p <- (ggplot(drop=FALSE, alpha=.6)</pre>
      + geom_density(aes(x=alpha, fill=distribution),
                     color=NA, alpha=.6,
                     data=prioralpha)
      #+ geom_density(aes(x=alpha, fill=distribution),
      #
                      color=NA, alpha=.6,
      #
                      data=postalpha)
      + ggtitle("Prior and posterior distributions of alpha\n")
      + scale_fill_discrete(drop=FALSE)
      + theme_bw()
      +xlim(0,10)
      +ylim(0, 1.3)
    )
р
```

```
}
# k-means comparison
plot(x=z[1,], y=z[2,], col=kmeans(t(z), centers=4)$cluster,
     xlab = "d = 1", ylab= "d = 2", main="k-means with K=4 clusters")
KM <- kmeans(t(z), centers=4)</pre>
dataKM <- data.frame("X"=z[1,], "Y"=z[2,],</pre>
                    "Cluster"=as.character(KM$cluster))
 dataCenters <- data.frame("X"=KM$centers[,1],</pre>
                           "Y"=KM$centers[,2],
                           "Cluster"=rownames(KM$centers))
p <- (ggplot(dataKM)</pre>
       + geom_point(aes(x=X, y=Y, col=Cluster))
       + geom_point(aes(x=X, y=Y, fill=Cluster, order=Cluster),
                    data=dataCenters, shape=22, size=5)
       + scale_colour_discrete(name="Cluster")
       + ggtitle("K-means with K=4 clusters\n"))
р
```

DPMGibbsN\_parallel

Slice Sampling of the Dirichlet Process Mixture Model with a prior on alpha

## **Description**

Slice Sampling of the Dirichlet Process Mixture Model with a prior on alpha

## Usage

```
DPMGibbsN_parallel(
  Ncpus,
  type_connec,
  z,
  hyperG0,
  a = 1e-04,
  b = 1e-04,
  N,
  doPlot = TRUE,
  nbclust_init = 30,
  plotevery = N/10,
```

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```
diagVar = TRUE,
  use_variance_hyperprior = TRUE,
  verbose = TRUE,
  monitorfile = "",
  ...
)
```

#### **Arguments**

Ncpus the number of processors available The type of connection between the processors. Supported cluster types are type\_connec "SOCK", "FORK", "MPI", and "NWS". See also makeCluster. data matrix d x n with d dimensions in rows and n observations in columns. z hyperG0 prior mixing distribution. shape hyperparameter of the Gamma prior on the concentration parameter of the а Dirichlet Process. Default is 0.0001. scale hyperparameter of the Gamma prior on the concentration parameter of the b Dirichlet Process. Default is 0.0001. If 0, then the concentration is fixed set to number of MCMC iterations. Ν doPlot logical flag indicating whether to plot MCMC iteration or not. Default to TRUE. number of clusters at initialization. Default to 30 (or less if there are less than nbclust\_init 30 observations). plotevery an integer indicating the interval between plotted iterations when doPlot is TRUE. diagVar logical flag indicating whether the variance of each cluster is estimated as a diagonal matrix, or as a full matrix. Default is TRUE (diagonal variance). use\_variance\_hyperprior logical flag indicating whether a hyperprior is added for the variance parameter. Default is TRUE which decrease the impact of the variance prior on the posterior. FALSE is useful for using an informative prior. verbose logical flag indicating whether partition info is written in the console at each MCMC iteration. monitorfile a writable connections or a character string naming a file to write into, to monitor the progress of the analysis. Default is "" which is no monitoring. See Details.

## Value

a object of class DPMclust with the following attributes:

mcmc\_partitions:

a list of length N. Each element mcmc\_partitions[n] is a vector of length n

additional arguments to be passed to plot\_DPM. Only used if doPlot is TRUE.

giving the partition of the n observations.

alpha: a vector of length N. cost[j] is the cost associated to partition c[[j]]

listU\_mu: a list of length N containing the matrices of mean vectors for all the mixture

components at each MCMC iteration

listU\_Sigma: a list of length N containing the arrays of covariances matrices for all the mixture

components at each MCMC iteration

U\_SS\_list: a list of length N containing the lists of sufficient statistics for all the mixture

components at each MCMC iteration

weights\_list: a list of length N containing the logposterior values at each MCMC iterations

logposterior\_list:

a list of length N containing the logposterior values at each MCMC iterations

data: the data matrix d x n with d dimensions in rows and n observations in columns

nb\_mcmcit: the number of MCMC iterations

clust\_distrib: the parametric distribution of the mixture component - "gaussian"

hyperG0: the prior on the cluster location

#### Author(s)

Boris Hejblum

#### See Also

**DPMGibbsN** 

```
# Scaling up: ----
rm(list=ls())
#Number of data
n <- 2000
set.seed(1234)
# Sample data
d <- 3
nclust <- 5
m <- matrix(nrow=d, ncol=nclust, runif(d*nclust)*8)</pre>
# p: cluster probabilities
p <- runif(nclust)</pre>
p \leftarrow p/sum(p)
# Covariance matrix of the clusters
sdev <- array(dim=c(d, d, nclust))</pre>
for (j in 1:nclust){
    sdev[, ,j] <- matrix(NA, nrow=d, ncol=d)</pre>
    diag(sdev[, ,j]) <- abs(rnorm(n=d, mean=0.3, sd=0.1))</pre>
    sdev[, ,j][lower.tri(sdev[, ,j], diag = FALSE)] <- rnorm(n=d*(d-1)/2,</pre>
    mean=0, sd=0.05)
    sdev[, ,j][upper.tri(sdev[, ,j], diag = FALSE)] <- (sdev[, ,j][</pre>
                                                        lower.tri(sdev[, ,j], diag = FALSE)])
}
```

```
c \leftarrow rep(0,n)
z <- matrix(0, nrow=d, ncol=n)</pre>
for(k in 1:n){
    c[k] = which(rmultinom(n=1, size=1, prob=p)!=0)
   z[,k] \leftarrow m[, c[k]] + sdev[, , c[k]]**matrix(rnorm(d, mean = 0, sd = 1), nrow=d, ncol=1)
    #cat(k, "/", n, " observations simulated\n", sep="")
}
# hyperprior on the Scale parameter of DPM
a <- 0.001
b <- 0.001
# Number of iterations
N <- 25
# do some plots
doPlot <- TRUE
# Set parameters of G0
hyperG0 <- list()</pre>
hyperG0[["mu"]] <- rep(0, d)
hyperG0[["kappa"]] <- 0.01
hyperG0[["nu"]] <- d + 2
hyperG0[["lambda"]] \leftarrow diag(d)/10
nbclust_init <- 30</pre>
if(interactive()){
 library(doParallel)
 MCMCsample <- DPMGibbsN_parallel(Ncpus=2, type_connec="FORK", z, hyperG0, a, b,
                                    N=1000, doPlot=FALSE, nbclust_init=30,
                                    plotevery=100, gg.add=list(ggplot2::theme_bw(),
                                    ggplot2::guides(shape =
                              ggplot2::guide_legend(override.aes = list(fill="grey45")))),
                                    diagVar=FALSE)
}
```

DPMGibbsN\_SeqPrior

Slice Sampling of Dirichlet Process Mixture of Gaussian distributions

## **Description**

Slice Sampling of Dirichlet Process Mixture of Gaussian distributions

## Usage

```
DPMGibbsN_SeqPrior(
```

```
z,
prior_inform,
hyperG0,
N,
nbclust_init,
add.vagueprior = TRUE,
weightnoninfo = NULL,
doPlot = TRUE,
plotevery = N/10,
diagVar = TRUE,
verbose = TRUE,
...
)
```

## **Arguments**

prior\_inform an informative prior such as the approximation computed by summary.DPMMclust.

hyperG0 a non informative prior component for the mixing distribution. Only used if add.vagueprior is TRUE.

N number of MCMC iterations.

nbclust\_init number of clusters at initialization. Default to 30 (or less if there are less than 30 observations).

add.vagueprior logical flag indicating whether a non informative component should be added to

the informative prior. Default is TRUE.

data matrix d x n with d dimensions in rows and n observations in columns.

the informative prior. Default is TROE.

weightnoninfo a real between 0 and 1 giving the weights of the non informative component in

the prior.

doPlot logical flag indicating whether to plot MCMC iteration or not. Default to TRUE.

plotevery an integer indicating the interval between plotted iterations when doPlot is

TRUE.

diagVar logical flag indicating whether the variance of each cluster is estimated as a

diagonal matrix, or as a full matrix. Default is TRUE (diagonal variance).

verbose logical flag indicating whether partition info is written in the console at each

MCMC iteration.

... additional arguments to be passed to plot\_DPM. Only used if doPlot is TRUE.

#### Value

a object of class DPMclust with the following attributes:

 ${\tt mcmc\_partitions:}$ 

a list of length N. Each element mcmc\_partitions[n] is a vector of length n

giving the partition of the n observations.

alpha: a vector of length N. cost[j] is the cost associated to partition c[[j]]

listU\_mu: a list of length N containing the matrices of mean vectors for all the mixture

components at each MCMC iteration

listU\_Sigma: a list of length N containing the arrays of covariances matrices for all the mixture

components at each MCMC iteration

U\_SS\_list: a list of length N containing the lists of sufficient statistics for all the mixture

components at each MCMC iteration

weights\_list:
logposterior\_list:

a list of length N containing the logposterior values at each MCMC iterations

data: the data matrix d x n with d dimensions in rows and n observations in columns.

nb\_mcmcit: the number of MCMC iterations

clust\_distrib: the parametric distribution of the mixture component - "gaussian"

hyperG0: the prior on the cluster location

#### Author(s)

Boris Hejblum, Chariff Alkhassim

## References

Hejblum BP, Alkhassim C, Gottardo R, Caron F and Thiebaut R (2019) Sequential Dirichlet Process Mixtures of Multivariate Skew t-distributions for Model-based Clustering of Flow Cytometry Data. The Annals of Applied Statistics, 13(1): 638-660. <doi: 10.1214/18-AOAS1209 <arXiv: 1702.04407 https://arxiv.org/abs/1702.04407 doi:10.1214/18AOAS1209

#### See Also

postProcess.DPMMclust DPMGibbsN

```
rm(list=ls())
library(NPflow)
#Number of data
n <- 1500
# Sample data
\#m \leftarrow matrix(nrow=2, ncol=4, c(-1, 1, 1.5, 2, 2, -2, 0.5, -2))
m \leftarrow matrix(nrow=2, ncol=4, c(-.8, .7, .5, .7, .5, -.7, -.5, -.7))
p <- c(0.2, 0.1, 0.4, 0.3) # frequence des clusters
sdev \leftarrow array(dim=c(2,2,4))
sdev[, ,1] \leftarrow matrix(nrow=2, ncol=2, c(0.3, 0, 0, 0.3))
sdev[, ,2] \leftarrow matrix(nrow=2, ncol=2, c(0.1, 0, 0, 0.3))
sdev[, ,3] <- matrix(nrow=2, ncol=2, c(0.3, 0.15, 0.15, 0.3))</pre>
sdev[, ,4] <- .3*diag(2)
c \leftarrow rep(0,n)
z <- matrix(0, nrow=2, ncol=n)</pre>
for(k in 1:n){
c[k] = which(rmultinom(n=1, size=1, prob=p)!=0)
z[,k] \leftarrow m[, c[k]] + sdev[, , c[k]]**matrix(rnorm(2, mean = 0, sd = 1), nrow=2, ncol=1)
```

```
\#cat(k, "/", n, " observations simulated\n", sep="")
d<-2
# Set parameters of G0
hyperG0 <- list()</pre>
hyperG0[["mu"]] <- rep(0,d)
hyperG0[["kappa"]] <- 0.001
hyperG0[["nu"]] <- d+2
hyperG0[["lambda"]] <- diag(d)/10</pre>
# hyperprior on the Scale parameter of DPM
a <- 0.0001
b <- 0.0001
# Number of iterations
N <- 30
# do some plots
doPlot <- TRUE
nbclust_init <- 20</pre>
## Data
########
library(ggplot2)
p \leftarrow (ggplot(data.frame("X"=z[1,], "Y"=z[2,]), aes(x=X, y=Y))
      + geom_point()
      + ggtitle("Toy example Data"))
p
if(interactive()){
# Gibbs sampler for Dirichlet Process Mixtures
MCMCsample <- DPMGibbsN(z, hyperG0, a, b, N=1500, doPlot, nbclust_init, plotevery=200,
                        gg.add=list(theme_bw(),
                        guides(shape=guide_legend(override.aes = list(fill="grey45")))),
                        diagVar=FALSE)
s <- summary(MCMCsample, posterior_approx=TRUE, burnin = 1000, thin=5)</pre>
F1 <- FmeasureC(pred=s$point_estim$c_est, ref=c)</pre>
F1
MCMCsample2 <- DPMGibbsN_SeqPrior(z, prior_inform=s$param_posterior,</pre>
                                  hyperG0, N=1500,
                                  add.vagueprior = TRUE,
                                  doPlot=TRUE, plotevery=100,
                                  nbclust_init=nbclust_init,
                                  gg.add=list(theme_bw(),
```

DPMGibbsSkewN

Slice Sampling of Dirichlet Process Mixture of skew normal distributions

## **Description**

Slice Sampling of Dirichlet Process Mixture of skew normal distributions

## Usage

```
DPMGibbsSkewN(
   z,
   hyperG0,
   a = 1e-04,
   b = 1e-04,
   N,
   doPlot = TRUE,
   nbclust_init = 30,
   plotevery = N/10,
   diagVar = TRUE,
   use_variance_hyperprior = TRUE,
   verbose = TRUE,
   ...
)
```

## Arguments

| Z       | data matrix d x n with d dimensions in rows and n observations in columns.  |
|---------|---|
| hyperG0 | prior mixing distribution.  |
| a       | shape hyperparameter of the Gamma prior on the concentration parameter of the Dirichlet Process. Default is $0.0001$ .  |
| b       | scale hyperparameter of the Gamma prior on the concentration parameter of the Dirichlet Process. Default is $0.0001$ . If $0$ , then the concentration is fixed set to a. |
| N       | number of MCMC iterations.  |
| doPlot  | logical flag indicating whether to plot MCMC iteration or not. Default to TRUE.   |

nbclust\_init number of clusters at initialization. Default to 30 (or less if there are less than

30 observations).

plotevery an integer indicating the interval between plotted iterations when doPlot is

TRUE.

diagVar logical flag indicating whether the variance of a cluster is a diagonal matrix.

Default is FALSE (full matrix).

use\_variance\_hyperprior

logical flag indicating whether a hyperprior is added for the variance parameter. Default is TRUE which decrease the impact of the variance prior on the posterior.

FALSE is useful for using an informative prior.

verbose logical flag indicating whether partition info is written in the console at each

MCMC iteration.

. . . additional arguments to be passed to plot\_DPMsn. Only used if doPlot is TRUE.

#### Value

a object of class DPMclust with the following attributes:

mcmc\_partitions:

a list of length N. Each element mcmc\_partitions[n] is a vector of length n

giving the partition of the n observations.

alpha: a vector of length N. cost[j] is the cost associated to partition c[[j]]

U\_SS\_list: a list of length N containing the lists of sufficient statistics for all the mixture

components at each MCMC iteration

weights\_list:

logposterior\_list:

a list of length N containing the logposterior values at each MCMC iterations

data: the data matrix d x n with d dimensions in rows and n observations in columns

nb mcmcit: the number of MCMC iterations

clust\_distrib: the parametric distribution of the mixture component - "skewnorm"

hyperG0: the prior on the cluster location

#### Author(s)

Boris Hejblum

#### References

Hejblum BP, Alkhassim C, Gottardo R, Caron F and Thiebaut R (2019) Sequential Dirichlet Process Mixtures of Multivariate Skew t-distributions for Model-based Clustering of Flow Cytometry Data. The Annals of Applied Statistics, 13(1): 638-660. <doi: 10.1214/18-AOAS1209 <arXiv: 1702.04407 https://arxiv.org/abs/1702.04407 doi:10.1214/18AOAS1209

```
rm(list=ls())
#Number of data
n <- 1000
set.seed(123)
d <- 2
ncl <- 4
# Sample data
sdev <- array(dim=c(d,d,ncl))</pre>
#xi <- matrix(nrow=d, ncol=ncl, c(-1.5, 1, 1.5, 1, 1.5, -2, -2, -2))
xi <- matrix(nrow=d, ncol=ncl, c(-0.5, 0, 0.5, 0, 0.5, -1, -1, 1))
##xi <- matrix(nrow=d, ncol=ncl, c(-0.3, 0, 0.5, 0.5, 0.5, -1.2, -1, 1))
psi <- matrix(nrow=d, ncol=4, c(0.4, -0.6, 0.8, 0, 0.3, -0.7, -0.3, -1.2))
p \leftarrow c(0.2, 0.1, 0.4, 0.3) # frequence des clusters
sdev[, ,1] \leftarrow matrix(nrow=d, ncol=d, c(0.3, 0, 0, 0.3))
sdev[, ,2] \leftarrow matrix(nrow=d, ncol=d, c(0.1, 0, 0, 0.3))
sdev[, ,3] <- matrix(nrow=d, ncol=d, c(0.3, 0.15, 0.15, 0.3))</pre>
sdev[, ,4] <- .3*diag(2)</pre>
c \leftarrow rep(0,n)
z <- matrix(0, nrow=d, ncol=n)</pre>
for(k in 1:n){
c[k] = which(rmultinom(n=1, size=1, prob=p)!=0)
sd = 1), nrow=d, ncol=1)
 \#cat(k, "/", n, " observations simulated\n", sep="")
}
# Set parameters of G0
hyperG0 <- list()</pre>
hyperG0[["b_xi"]] <- rep(0,d)
hyperG0[["b_psi"]] <- rep(0,d)
hyperG0[["kappa"]] <- 0.0001
hyperG0[["D_xi"]] <- 100
hyperG0[["D_psi"]] <- 100
hyperG0[["nu"]] <- d + 1
hyperG0[["lambda"]] <- diag(d)</pre>
 # hyperprior on the Scale parameter of DPM
 a <- 0.0001
 b <- 0.0001
 # do some plots
 doPlot <- TRUE
 nbclust_init <- 30</pre>
```

```
## Data
#######
library(ggplot2)
p \leftarrow (ggplot(data.frame("X"=z[1,], "Y"=z[2,]), aes(x=X, y=Y))
      + geom_point()
      + ggtitle("Simple example in 2d data")
      +xlab("D1")
      +ylab("D2")
      +theme_bw())
р
c2plot <- factor(c)</pre>
levels(c2plot) <- c("3", "2", "4", "1")
pp <- (ggplot(data.frame("X"=z[1,], "Y"=z[2,], "Cluster"=as.character(c2plot)))</pre>
      + geom_point(aes(x=X, y=Y, colour=Cluster, fill=Cluster))
      + ggtitle("Slightly overlapping skew-normal simulation\n")
      + xlab("D1")
      + ylab("D2")
      + theme_bw()
    + scale_colour_discrete(guide=guide_legend(override.aes = list(size = 6, shape=22))))
pp
## alpha priors plots
#######################
prioralpha <- data.frame("alpha"=rgamma(n=5000, shape=a, scale=1/b),</pre>
                         "distribution" =factor(rep("prior",5000),
                        levels=c("prior", "posterior")))
p <- (ggplot(prioralpha, aes(x=alpha))</pre>
      + geom_histogram(aes(y=..density..),
                        colour="black", fill="white")
      + geom_density(alpha=.2, fill="red")
      + ggtitle(paste("Prior distribution on alpha: Gamma(", a,
                 ",", b, ")\n", sep=""))
     )
p
if(interactive()){
# Gibbs sampler for Dirichlet Process Mixtures
MCMCsample_sn <- DPMGibbsSkewN(z, hyperG0, a, b, N=2500,</pre>
                                doPlot, nbclust_init, plotevery=200,
                                gg.add=list(theme_bw(),
                        guides(shape=guide_legend(override.aes = list(fill="grey45")))),
                               diagVar=FALSE)
s <- summary(MCMCsample_sn, burnin = 2000, thin=10)</pre>
#cluster_est_binder(MCMCsample_sn$mcmc_partitions[1000:1500])
print(s)
```

```
plot(s)
#plot_ConvDPM(MCMCsample_sn, from=2)
# k-means
plot(x=z[1,], y=z[2,], col=kmeans(t(z), centers=4)$cluster,
     xlab = "d = 1", ylab= "d = 2", main="k-means with K=4 clusters")
KM <- kmeans(t(z), centers=4)</pre>
KMclust <- factor(KM$cluster)</pre>
levels(KMclust) <- c("2", "4", "1", "3")</pre>
dataKM <- data.frame("X"=z[1,], "Y"=z[2,],</pre>
                    "Cluster"=as.character(KMclust))
dataCenters <- data.frame("X"=KM$centers[,1],</pre>
                           "Y"=KM$centers[,2],
                           "Cluster"=c("2", "4", "1", "3"))
p <- (ggplot(dataKM)</pre>
      + geom_point(aes(x=X, y=Y, col=Cluster))
      + geom_point(aes(x=X, y=Y, fill=Cluster, order=Cluster),
                    data=dataCenters, shape=22, size=5)
      + scale_colour_discrete(name="Cluster",
                               guide=guide_legend(override.aes=list(size=6, shape=22)))
      + ggtitle("K-means with K=4 clusters\n")
      + theme_bw()
)
postalpha <- data.frame("alpha"=MCMCsample_sn$alpha[501:1000],</pre>
                         "distribution" = factor(rep("posterior",1000-500),
                         levels=c("prior", "posterior")))
postK <- data.frame("K"=sapply(lapply(postalpha$alpha, "["),</pre>
                                function(x)\{sum(x/(x+0:(1000-1)))\})
p <- (ggplot(postalpha, aes(x=alpha))</pre>
      + geom_histogram(aes(y=..density..), binwidth=.1,
                        colour="black", fill="white")
      + geom_density(alpha=.2, fill="blue")
      + ggtitle("Posterior distribution of alpha\n")
      # Ignore NA values for mean
      # Overlay with transparent density plot
      + geom_vline(aes(xintercept=mean(alpha, na.rm=T)),
                    color="red", linetype="dashed", size=1)
    )
р
```

```
p <- (ggplot(postK, aes(x=K))</pre>
       + geom_histogram(aes(y=..density..),
                         colour="black", fill="white")
       + geom_density(alpha=.2, fill="blue")
       + ggtitle("Posterior distribution of predicted K\n")
       # Ignore NA values for mean
       # Overlay with transparent density plot
       + geom_vline(aes(xintercept=mean(K, na.rm=T)),
                     color="red", linetype="dashed", size=1)
       #+ scale_x_continuous(breaks=c(0:6)*2, minor_breaks=c(0:6)*2+1)
       + scale_x_continuous(breaks=c(1:12))
     )
 р
 p <- (ggplot(drop=FALSE, alpha=.6)</pre>
       + geom_density(aes(x=alpha, fill=distribution),
                       color=NA, alpha=.6,
                       data=postalpha)
       + geom_density(aes(x=alpha, fill=distribution),
                       color=NA, alpha=.6,
                       data=prioralpha)
       + ggtitle("Prior and posterior distributions of alpha\n")
       + scale_fill_discrete(drop=FALSE)
       + theme_bw()
       + xlim(0,100)
     )
 р
#Skew Normal
n=100000
xi <- 0
d <- 0.995
alpha <- d/sqrt(1-d^2)</pre>
z <- rtruncnorm(n,a=0, b=Inf)</pre>
e <- rnorm(n, mean = 0, sd = 1)
x <- d*z + sqrt(1-d^2)*e
o <- 1
y <- xi+o*x
nu=1.3
w <- rgamma(n,scale=nu/2, shape=nu/2)
yy <- xi+o*x/w
snd <- data.frame("Y"=y,"YY"=yy)</pre>
p \leftarrow (ggplot(snd)+geom\_density(aes(x=Y), fill="blue", alpha=.2)
     + theme_bw()
     + ylab("Density")
     + ggtitle("Y~SN(0,1,10)\n")
     + xlim(-1,6)
     + ylim(0,0.8)
     )
p <- (ggplot(snd)+geom_density(aes(x=YY), fill="blue", alpha=.2)</pre>
     + theme_bw()
```

```
+ ylab("Density")
     + ggtitle("Y~ST(0,1,10,1.3)\n")
     + xlim(-2,40)
     + ylim(0,0.8)
     )
p <- (ggplot(snd)</pre>
     + geom_density(aes(x=Y, fill="blue"), alpha=.2)
     + geom_density(aes(x=YY, fill="red"), alpha=.2)
     + theme_bw()
     +theme(legend.text = element_text(size = 13), legend.position="bottom")
     + ylab("Density")
     + xlim(-2,40)
     + ylim(0,0.8)
     + scale_fill_manual(name="", labels=c("Y~SN(0,1,10)
                                                                    ", "Y~ST(0,1,10,1.3)"),
     guide="legend", values=c("blue", "red"))
     )
р
#Variations
n=100000
xi <- -1
d <- 0.995
alpha <- d/sqrt(1-d^2)
z <- rtruncnorm(n,a=0, b=Inf)</pre>
e <- rnorm(n, mean = 0, sd = 1)
x \leftarrow d*z + sqrt(1-d^2)*e
snd <- data.frame("X"=x)</pre>
p \leftarrow (ggplot(snd)+geom\_density(aes(x=X), fill="blue", alpha=.2)
     + theme_bw()
     + ylab("Density")
     + ggtitle("X~SN(10)\n")
     + xlim(-1.5,4)
     + ylim(0,1.6)
     )
р
o <- 0.5
y \leftarrow xi + o * x
snd <- data.frame("Y"=y)</pre>
p \leftarrow (ggplot(snd)+geom\_density(aes(x=Y), fill="blue", alpha=.2)
     + theme_bw()
     + ylab("Density")
     + ggtitle("Y~SN(-1,1,10)\n")
     + xlim(-1.5,4)
     + ylim(0,1.6)
p
```

```
#Simple toy example
n <- 500
set.seed(12345)
d < - 2
ncl <- 4
# Sample data
sdev <- array(dim=c(d,d,ncl))</pre>
xi <- matrix(nrow=d, ncol=ncl, c(-1.5, 1, 1.5, 1, 1.5, -2, -2, -2))
psi <- matrix(nrow=d, ncol=4, c(0.4, -0.6, 0.8, 0, 0.3, -0.7, -0.3, -1.2))
p <- c(0.2, 0.1, 0.4, 0.3) # frequence des clusters
sdev[, ,1] \leftarrow matrix(nrow=d, ncol=d, c(0.3, 0, 0, 0.3))
sdev[, ,2] \leftarrow matrix(nrow=d, ncol=d, c(0.1, 0, 0, 0.3))
sdev[, ,3] \leftarrow matrix(nrow=d, ncol=d, c(0.3, 0.15, 0.15, 0.3))
sdev[, ,4] <- .3*diag(2)
#' # Set parameters of G0
hyperG0 <- list()</pre>
hyperG0[["b_xi"]] <- rep(0,d)
hyperG0[["b_psi"]] \leftarrow rep(0,d)
hyperG0[["kappa"]] <- 0.0001
hyperG0[["D_xi"]] <- 100
hyperG0[["D_psi"]] <- 100
hyperG0[["nu"]] <- d + 1
hyperG0[["lambda"]] <- diag(d)</pre>
c \leftarrow rep(0,n)
z <- matrix(0, nrow=d, ncol=n)</pre>
for(k in 1:n){
c[k] = which(rmultinom(n=1, size=1, prob=p)!=0)
z[,k] \leftarrow xi[, c[k]] + psi[, c[k]]*abs(rnorm(1)) + sdev[, , c[k]]%*%matrix(rnorm(d, mean = 0, local context)) + sdev[, local context)]
                                                                      sd = 1), nrow=d, ncol=1)
cat(k, "/", n, " observations simulated\n", sep="")
 MCMCsample\_sn\_sep <- DPMGibbsSkewN(z, hyperG0, a, b, N=600,
                                       doPlot, nbclust_init, plotevery=100,
                                       gg.add=list(theme_bw(),
                          guides(shape=guide_legend(override.aes = list(fill="grey45")))),
                                       diagVar=TRUE)
 s <- summary(MCMCsample_sn, burnin = 400)</pre>
}
```

```
DPMGibbsSkewN_parallel
```

Parallel Implementation of Slice Sampling of Dirichlet Process Mixture of skew normal distributions

## Description

If the monitorfile argument is a character string naming a file to write into, in the case of a new file that does not exist yet, such a new file will be created. A line is written at each MCMC iteration.

## Usage

```
DPMGibbsSkewN_parallel(
  Ncpus,
  type_connec,
 Ζ,
  hyperG0,
  a = 1e-04,
  b = 1e-04,
 Ν,
  doPlot = FALSE,
  nbclust_init = 30,
 plotevery = N/10,
  diagVar = TRUE,
  use_variance_hyperprior = TRUE,
  verbose = FALSE,
 monitorfile = "",
)
```

## **Arguments**

| Ncpus       | the number of processors available  |
|-------------|---|
| type_connec | The type of connection between the processors. Supported cluster types are "SOCK", "FORK", "MPI", and "NWS". See also makeCluster.  |
| Z           | data matrix $d \times n$ with $d$ dimensions in rows and $n$ observations in columns.   |
| hyperG0     | prior mixing distribution.  |
| а           | shape hyperparameter of the Gamma prior on the concentration parameter of the Dirichlet Process. Default is 0.0001.   |
| b           | scale hyperparameter of the Gamma prior on the concentration parameter of the Dirichlet Process. Default is $0.0001$ . If $0$ , then the concentration is fixed set to a. |
| N           | number of MCMC iterations.  |
| doPlot      | logical flag indicating whether to plot MCMC iteration or not. Default to TRUE.   |

nbclust\_init number of clusters at initialization. Default to 30 (or less if there are less than

30 observations).

plotevery an integer indicating the interval between plotted iterations when doPlot is

TRUE.

diagVar logical flag indicating whether the variance of each cluster is estimated as a

diagonal matrix, or as a full matrix. Default is TRUE (diagonal variance).

use\_variance\_hyperprior

logical flag indicating whether a hyperprior is added for the variance parameter. Default is TRUE which decrease the impact of the variance prior on the posterior.

FALSE is useful for using an informative prior.

verbose logical flag indicating whether partition info is written in the console at each

MCMC iteration.

monitorfile a writable connections or a character string naming a file to write into, to monitor

the progress of the analysis. Default is "" which is no monitoring. See Details.

... additional arguments to be passed to plot\_DPM. Only used if doPlot is TRUE.

#### Value

a object of class DPMclust with the following attributes:

mcmc\_partitions:

a list of length N. Each element  $mcmc\_partitions[n]$  is a vector of length n

giving the partition of the n observations.

alpha: a vector of length N. cost[j] is the cost associated to partition c[[j]]

U\_SS\_list: a list of length N containing the lists of sufficient statistics for all the mixture

components at each MCMC iteration

weights\_list:

logposterior\_list:

a list of length N containing the logposterior values at each MCMC iterations

data: the data matrix d x n with d dimensions in rows and n observations in columns

nb\_mcmcit: the number of MCMC iterations

clust\_distrib: the parametric distribution of the mixture component - "skewnorm"

hyperG0: the prior on the cluster location

## Author(s)

Boris Hejblum

#### References

Hejblum BP, Alkhassim C, Gottardo R, Caron F and Thiebaut R (2019) Sequential Dirichlet Process Mixtures of Multivariate Skew t-distributions for Model-based Clustering of Flow Cytometry Data. The Annals of Applied Statistics, 13(1): 638-660. <doi: 10.1214/18-AOAS1209 <arXiv: 1702.04407 https://arxiv.org/abs/1702.04407 doi:10.1214/18AOAS1209

```
rm(list=ls())
#Number of data
n <- 2000
set.seed(1234)
d <- 4
ncl <- 5
# Sample data
sdev <- array(dim=c(d,d,ncl))</pre>
xi <- matrix(nrow=d, ncol=ncl, c(runif(n=d*ncl,min=0,max=3)))</pre>
psi <- matrix(nrow=d, ncol=ncl, c(runif(n=d*ncl,min=-1,max=1)))</pre>
p <- runif(n=ncl)</pre>
p \leftarrow p/sum(p)
sdev0 <- diag(runif(n=d, min=0.05, max=0.6))</pre>
for (j in 1:ncl){
     sdev[, ,j] \leftarrow invwishrnd(n = d+2, lambda = sdev0)
}
c \leftarrow rep(0,n)
z <- matrix(0, nrow=d, ncol=n)</pre>
for(k in 1:n){
c[k] = which(rmultinom(n=1, size=1, prob=p)!=0)
sd = 1), nrow=d, ncol=1)
 #cat(k, "/", n, " observations simulated\n", sep="")
}
# Set parameters of G0
hyperG0 <- list()</pre>
hyperG0[["b_xi"]] <- rep(0,d)
hyperG0[["b_psi"]] \leftarrow rep(0,d)
hyperG0[["kappa"]] <- 0.001
hyperG0[["D_xi"]] <- 100
hyperG0[["D_psi"]] <- 100
hyperG0[["nu"]] <- d + 1
hyperG0[["lambda"]] <- diag(d)/10</pre>
 # hyperprior on the Scale parameter of DPM
 a <- 0.0001
 b <- 0.0001
 # do some plots
 doPlot <- TRUE
 nbclust_init <- 30</pre>
 z <- z*200
```

```
## Data
########
library(ggplot2)
p \leftarrow (ggplot(data.frame("X"=z[1,], "Y"=z[2,]), aes(x=X, y=Y))
      + geom_point()
      + ggtitle("Simple example in 2d data")
      +xlab("D1")
      +ylab("D2")
      +theme_bw())
р
## alpha priors plots
######################
prioralpha <- data.frame("alpha"=rgamma(n=5000, shape=a, scale=1/b),</pre>
                        "distribution" =factor(rep("prior",5000),
                        levels=c("prior", "posterior")))
p <- (ggplot(prioralpha, aes(x=alpha))</pre>
      + geom_histogram(aes(y=..density..),
                       colour="black", fill="white")
      + geom_density(alpha=.2, fill="red")
      + ggtitle(paste("Prior distribution on alpha: Gamma(", a,
                ",", b, ")\n", sep=""))
p
# Gibbs sampler for Dirichlet Process Mixtures
if(interactive()){
 MCMCsample_sn_par <- DPMGibbsSkewN_parallel(Ncpus=parallel::detectCores()-1,</pre>
                                             type_connec="SOCK", z, hyperG0,
                                             a, b, N=5000, doPlot, nbclust_init,
                                             plotevery=25, gg.add=list(theme_bw(),
                        guides(shape=guide_legend(override.aes = list(fill="grey45")))))
 plot_ConvDPM(MCMCsample_sn_par, from=2)
}
```

DPMGibbsSkewT

Slice Sampling of Dirichlet Process Mixture of skew Student's t-distributions

## **Description**

Slice Sampling of Dirichlet Process Mixture of skew Student's t-distributions

## Usage

```
DPMGibbsSkewT(
  hyperG0,
  a = 1e-04,
  b = 1e-04,
 Ν,
  doPlot = TRUE.
  nbclust_init = 30,
 plotevery = N/10,
  diagVar = TRUE,
  use_variance_hyperprior = TRUE,
  verbose = TRUE,
)
```

# **Arguments** Z

data matrix d x n with d dimensions in rows and n observations in columns.

parameters of the prior mixing distribution in a list with the following named components:

• "b\_xi": a vector of length d with the mean location prior parameter. Can be set as the empirical mean of the data in an Empirical Bayes fashion.

- "b\_psi": a vector of length d with the skewness location prior parameter. Can be set as 0 a priori.
- "kappa": a strictly positive number part of the inverse-Wishart component of the prior on the variance matrix. Can be set as very small (e.g. 0.001) a priori.
- "D\_xi": hyperprior controlling the information in  $\xi$  (the larger the less information is carried). 100 is a reasonable value, based on Fruhwirth-Schnatter et al., Biostatistics, 2010.
- "D\_psi": hyperprior controlling the information in  $\psi$  (the larger the less information is carried). 100 is a reasonable value, based on Fruhwirth-Schnatter et al., Biostatistics, 2010
- "nu": a prior number on the degrees of freedom of the t component that must be strictly greater than d. Can be set as d + 1 for instance.
- "lambda": a d x d symmetric definitive positive matrix part of the inverse-Wishart component of the prior on the variance matrix. Can be set as the diagonal of empirical variance of the data in an Empircal Bayes fashion divided by a factor 3 according to Fruhwirth-Schnatter et al., Biostatistics, 2010.

shape hyperparameter of the Gamma prior on the concentration parameter of the Dirichlet Process. Default is 0.0001.

scale hyperparameter of the Gamma prior on the concentration parameter of the Dirichlet Process. Default is 0.0001. If 0, then the concentration is fixed set to a.

hyperG0

а

b

N number of MCMC iterations.

doPlot logical flag indicating whether to plot MCMC iteration or not. Default to TRUE.

nbclust\_init number of clusters at initialization. Default to 30 (or less if there are less than

30 observations).

plotevery an integer indicating the interval between plotted iterations when doPlot is

TRUE.

diagVar logical flag indicating whether the variance of each cluster is estimated as a

diagonal matrix, or as a full matrix. Default is TRUE (diagonal variance).

use\_variance\_hyperprior

logical flag indicating whether a hyperprior is added for the variance parameter. Default is TRUE which decrease the impact of the variance prior on the posterior.

FALSE is useful for using an informative prior.

verbose logical flag indicating whether partition info is written in the console at each

MCMC iteration.

... additional arguments to be passed to plot\_DPMst. Only used if doPlot is TRUE.

#### Value

a object of class DPMclust with the following attributes:

mcmc\_partitions:

a list of length N. Each element mcmc\_partitions[n] is a vector of length n

giving the partition of the n observations.

alpha: a vector of length N. cost[j] is the cost associated to partition c[[j]]

U\_SS\_list: a list of length N containing the lists of sufficient statistics for all the mixture

components at each MCMC iteration

weights\_list: a list of length N containing the weights of each mixture component for each

MCMC iterations

logposterior\_list:

a list of length N containing the logposterior values at each MCMC iterations

data: the data matrix d x n with d dimensions in rows and n observations in columns

nb\_mcmcit: the number of MCMC iterations

clust\_distrib:

the parametric distribution of the mixture component - "skewt"

hyperG0: the prior on the cluster location

#### Author(s)

Boris Heiblum

#### References

Hejblum BP, Alkhassim C, Gottardo R, Caron F and Thiebaut R (2019) Sequential Dirichlet Process Mixtures of Multivariate Skew t-distributions for Model-based Clustering of Flow Cytometry Data. The Annals of Applied Statistics, 13(1): 638-660. <doi: 10.1214/18-AOAS1209> <arXiv: 1702.04407> https://arxiv.org/abs/1702.04407 doi:10.1214/18AOAS1209

Fruhwirth-Schnatter S, Pyne S, Bayesian inference for finite mixtures of univariate and multivariate skew-normal and skew-t distributions, Biostatistics, 2010.

```
rm(list=ls())
#Number of data
n <- 2000
set.seed(4321)
d <- 2
ncl <- 4
# Sample data
library(truncnorm)
sdev <- array(dim=c(d,d,ncl))</pre>
#xi <- matrix(nrow=d, ncol=ncl, c(-1.5, 1.5, 1.5, 1.5, 2, -2.5, -2.5, -3))</pre>
#xi <- matrix(nrow=d, ncol=ncl, c(-0.5, 0, 0.5, 0, 0.5, -1, -1, 1))</pre>
xi <- matrix(nrow=d, ncol=ncl, c(-0.2, 0.5, 2.4, 0.4, 0.6, -1.3, -0.9, -2.7))
psi \leftarrow matrix(nrow=d, ncol=4, c(0.3, -0.7, -0.8, 0, 0.3, -0.7, 0.2, 0.9))
nu < -c(100, 25, 8, 5)
p <- c(0.15, 0.05, 0.5, 0.3) # frequence des clusters
sdev[, ,1] \leftarrow matrix(nrow=d, ncol=d, c(0.3, 0, 0, 0.3))
sdev[, ,2] \leftarrow matrix(nrow=d, ncol=d, c(0.1, 0, 0, 0.3))
sdev[, ,3] <- matrix(nrow=d, ncol=d, c(0.3, 0.15, 0.15, 0.3))</pre>
sdev[, ,4] <- .3*diag(2)
c \leftarrow rep(0,n)
w <- rep(1,n)
z <- matrix(0, nrow=d, ncol=n)</pre>
for(k in 1:n){
 c[k] = which(rmultinom(n=1, size=1, prob=p)!=0)
 w[k] \leftarrow rgamma(1, shape=nu[c[k]]/2, rate=nu[c[k]]/2)
z[,k] \leftarrow xi[, c[k]] + psi[, c[k]]*rtruncnorm(n=1, a=0, b=Inf, mean=0, sd=1/sqrt(w[k])) +
            (sdev[, , c[k]]/sqrt(w[k]))%*%matrix(rnorm(d, mean = 0, sd = 1), nrow=d, ncol=1)
 #cat(k, "/", n, " observations simulated\n", sep="")
}
# Set parameters of G0
hyperG0 <- list()</pre>
hyperG0[["b_xi"]] <- rowMeans(z)</pre>
hyperG0[["b_psi"]] \leftarrow rep(0,d)
hyperG0[["kappa"]] <- 0.001
hyperG0[["D_xi"]] <- 100
hyperG0[["D_psi"]] <- 100
hyperG0[["nu"]] <- d+1
hyperG0[["lambda"]] <- diag(apply(z,MARGIN=1, FUN=var))/3
 # hyperprior on the Scale parameter of DPM
 a <- 0.0001
 b <- 0.0001
```

```
## Data
########
library(ggplot2)
p <- (ggplot(data.frame("X"=z[1,], "Y"=z[2,]), aes(x=X, y=Y))</pre>
      + geom_point()
      #+ ggtitle("Simple example in 2d data")
      +xlab("D1")
      +ylab("D2")
      +theme_bw())
p #pdf(height=8.5, width=8.5)
c2plot <- factor(c)</pre>
levels(c2plot) <- c("4", "1", "3", "2")
pp <- (ggplot(data.frame("X"=z[1,], "Y"=z[2,], "Cluster"=as.character(c2plot)))</pre>
      + geom_point(aes(x=X, y=Y, colour=Cluster, fill=Cluster))
      #+ ggtitle("Slightly overlapping skew-normal simulation\n")
      + xlab("D1")
      + ylab("D2")
      + theme_bw()
    + scale_colour_discrete(guide=guide_legend(override.aes = list(size = 6, shape=22))))
pp #pdf(height=7, width=7.5)
## alpha priors plots
#############################
prioralpha <- data.frame("alpha"=rgamma(n=5000, shape=a, scale=1/b),</pre>
                         "distribution" =factor(rep("prior",5000),
                        levels=c("prior", "posterior")))
p <- (ggplot(prioralpha, aes(x=alpha))</pre>
      + geom_histogram(aes(y=..density..),
                        colour="black", fill="white")
      + geom_density(alpha=.2, fill="red")
      + ggtitle(paste("Prior distribution on alpha: Gamma(", a,
                 ",", b, ")\n", sep=""))
     )
р
if(interactive()){
# Gibbs sampler for Dirichlet Process Mixtures
MCMCsample_st <- DPMGibbsSkewT(z, hyperG0, a, b, N=1500,</pre>
                                doPlot=TRUE, nbclust_init=30, plotevery=100,
                               diagVar=FALSE)
s <- summary(MCMCsample_st, burnin = 1000, thin=10, lossFn = "Binder")</pre>
print(s)
plot(s, hm=TRUE) #pdf(height=8.5, width=10.5) #png(height=700, width=720)
plot_ConvDPM(MCMCsample_st, from=2)
#cluster_est_binder(MCMCsample_st$mcmc_partitions[900:1000])
```

}

```
DPMGibbsSkewT_parallel
```

Slice Sampling of Dirichlet Process Mixture of skew Student's t-distributions

# Description

Slice Sampling of Dirichlet Process Mixture of skew Student's t-distributions

# Usage

```
DPMGibbsSkewT_parallel(
 Ncpus,
  type_connec,
 Ζ,
 hyperG0,
 a = 1e-04,
 b = 1e-04,
 N,
  doPlot = FALSE,
  nbclust_init = 30,
 plotevery = N/10,
 diagVar = TRUE,
  use_variance_hyperprior = TRUE,
 verbose = FALSE,
 monitorfile = "",
)
```

# Arguments

| Ncpus       | the number of processors available  |
|-------------|---|
| type_connec | The type of connection between the processors. Supported cluster types are "PSOCK", "FORK", "SOCK", "MPI", and "NWS". See also makeCluster.                               |
| z           | data matrix d x n with d dimensions in rows and n observations in columns.  |
| hyperG0     | prior mixing distribution.  |
| a           | shape hyperparameter of the Gamma prior on the concentration parameter of the Dirichlet Process. Default is $0.0001$ .  |
| b           | scale hyperparameter of the Gamma prior on the concentration parameter of the Dirichlet Process. Default is $0.0001$ . If $0$ , then the concentration is fixed set to a. |
| N           | number of MCMC iterations.  |

doPlot logical flag indicating whether to plot MCMC iteration or not. Default to TRUE.

nbclust\_init number of clusters at initialization. Default to 30 (or less if there are less than

30 observations).

plotevery an integer indicating the interval between plotted iterations when doPlot is

TRUE.

diagVar logical flag indicating whether the variance of each cluster is estimated as a

diagonal matrix, or as a full matrix. Default is TRUE (diagonal variance).

use\_variance\_hyperprior

logical flag indicating whether a hyperprior is added for the variance parameter. Default is TRUE which decrease the impact of the variance prior on the posterior.

FALSE is useful for using an informative prior.

verbose logical flag indicating whether partition info is written in the console at each

MCMC iteration.

monitorfile a writable connections or a character string naming a file to write into, to monitor

the progress of the analysis. Default is "" which is no monitoring. See Details.

... additional arguments to be passed to plot\_DPMst. Only used if doPlot is TRUE.

#### Value

a object of class DPMclust with the following attributes:

mcmc\_partitions:

a list of length N. Each element mcmc\_partitions[n] is a vector of length n

giving the partition of the n observations.

alpha: a vector of length N. cost[j] is the cost associated to partition c[[j]]

U\_SS\_list: a list of length N containing the lists of sufficient statistics for all the mixture

components at each MCMC iteration

weights\_list: a list of length N containing the weights of each mixture component for each

MCMC iterations

logposterior\_list:

a list of length N containing the logposterior values at each MCMC iterations

data: the data matrix d x n with d dimensions in rows and n observations in columns

nb\_mcmcit: the number of MCMC iterations

clust\_distrib: the parametric distribution of the mixture component - "skewt"

hyperG0: the prior on the cluster location

## Author(s)

Boris Hejblum

#### References

Hejblum BP, Alkhassim C, Gottardo R, Caron F and Thiebaut R (2019) Sequential Dirichlet Process Mixtures of Multivariate Skew t-distributions for Model-based Clustering of Flow Cytometry Data. The Annals of Applied Statistics, 13(1): 638-660. <doi: 10.1214/18-AOAS1209 <arXiv: 1702.04407 https://arxiv.org/abs/1702.04407 doi:10.1214/18AOAS1209

```
rm(list=ls())
#Number of data
n <- 2000
set.seed(123)
#set.seed(4321)
d <- 2
ncl <- 4
# Sample data
sdev <- array(dim=c(d,d,ncl))</pre>
xi <- matrix(nrow=d, ncol=ncl, c(-1.5, 1, 1.5, 1, 1.5, -2, -2, -2))
psi <- matrix(nrow=d, ncol=4, c(0.4, -0.6, 0.8, 0, 0.3, -0.7, -0.3, -0.8))
p <- c(0.2, 0.1, 0.4, 0.3) # frequence des clusters
sdev[, ,1] \leftarrow matrix(nrow=d, ncol=d, c(0.3, 0, 0, 0.3))
sdev[, ,2] \leftarrow matrix(nrow=d, ncol=d, c(0.1, 0, 0, 0.3))
sdev[, ,3] <- matrix(nrow=d, ncol=d, c(0.3, 0.15, 0.15, 0.3))</pre>
sdev[, ,4] <- .3*diag(2)</pre>
c \leftarrow rep(0,n)
z <- matrix(0, nrow=d, ncol=n)</pre>
for(k in 1:n){
c[k] = which(rmultinom(n=1, size=1, prob=p)!=0)
 z[,k] \leftarrow (xi[, c[k]]
          + psi[, c[k]]*abs(rnorm(1))
          + sdev[, , c[k]]%*%matrix(rnorm(d, mean = 0, sd = 1), nrow=d, ncol=1))
 #cat(k, "/", n, " observations simulated\n", sep="")
# Set parameters of G0
hyperG0 <- list()</pre>
hyperG0[["b_xi"]] <- rep(0,d)
hyperG0[["b_psi"]] <- rep(0,d)
hyperG0[["kappa"]] <- 0.001
hyperG0[["D_xi"]] <- 100
hyperG0[["D_psi"]] <- 100
hyperG0[["nu"]] <- d + 1
hyperG0[["lambda"]] <- diag(d)</pre>
 # hyperprior on the Scale parameter of DPM
 a <- 0.0001
 b <- 0.0001
 # do some plots
 doPlot <- TRUE
 nbclust_init <- 30</pre>
```

```
## Data
########
library(ggplot2)
p \leftarrow (ggplot(data.frame("X"=z[1,], "Y"=z[2,]), aes(x=X, y=Y))
      + geom_point()
      + ggtitle("Simple example in 2d data")
      +xlab("D1")
      +ylab("D2")
      +theme_bw())
р
c2plot <- factor(c)</pre>
levels(c2plot) <- c("3", "2", "4", "1")
pp <- (ggplot(data.frame("X"=z[1,], "Y"=z[2,], "Cluster"=as.character(c2plot)))</pre>
      + geom_point(aes(x=X, y=Y, colour=Cluster, fill=Cluster))
      + ggtitle("Slightly overlapping skew-normal simulation\n")
      + xlab("D1")
      + ylab("D2")
      + theme_bw()
    + scale_colour_discrete(guide=guide_legend(override.aes = list(size = 6, shape=22))))
pp
## alpha priors plots
############################
prioralpha <- data.frame("alpha"=rgamma(n=5000, shape=a, scale=1/b),</pre>
                         "distribution" =factor(rep("prior",5000),
                         levels=c("prior", "posterior")))
p <- (ggplot(prioralpha, aes(x=alpha))</pre>
      + geom_histogram(aes(y=..density..),
                        colour="black", fill="white")
      + geom_density(alpha=.2, fill="red")
      + ggtitle(paste("Prior distribution on alpha: Gamma(", a,
                 ",", b, ")\n", sep=""))
     )
р
if(interactive()){
# Gibbs sampler for Dirichlet Process Mixtures
MCMCsample_st <- DPMGibbsSkewT(z, hyperG0, a, b, N=2000,</pre>
                            doPlot, nbclust_init, plotevery=100, gg.add=list(theme_bw(),
                        guides(shape=guide_legend(override.aes = list(fill="grey45")))),
                                diagVar=FALSE)
s <- summary(MCMCsample_st, burnin = 350)</pre>
print(s)
plot(s)
plot_ConvDPM(MCMCsample_st, from=2)
cluster_est_binder(MCMCsample_st$mcmc_partitions[1500:2000])
```

}

```
DPMGibbsSkewT_SeqPrior
```

Slice Sampling of Dirichlet Process Mixture of skew Student's t-distributions

# Description

Slice Sampling of Dirichlet Process Mixture of skew Student's t-distributions

# Usage

```
DPMGibbsSkewT_SeqPrior(
   z,
   prior_inform,
   hyperG0,
   N,
   nbclust_init,
   add.vagueprior = TRUE,
   weightnoninfo = NULL,
   doPlot = TRUE,
   plotevery = N/10,
   diagVar = TRUE,
   verbose = TRUE,
   ...
)
```

## **Arguments**

| z              | data matrix d x n with d dimensions in rows and n observations in columns.   |
|----------------|--|
| prior_inform   | an informative prior such as the approximation computed by ${\tt summary.DPMMclust.}$                                  |
| hyperG0        | prior mixing distribution.   |
| N              | number of MCMC iterations.   |
| nbclust_init   | number of clusters at initialization. Default to 30 (or less if there are less than 30 observations).                  |
| add.vagueprior | logical flag indicating whether a non informative component should be added to the informative prior. Default is TRUE. |
| weightnoninfo  | a real between 0 and 1 giving the weights of the non informative component in the prior.                               |
| doPlot         | logical flag indicating whether to plot MCMC iteration or not. Default to TRUE.  |

plotevery an integer indicating the interval between plotted iterations when doPlot is

TRUE.

diagVar logical flag indicating whether the variance of each cluster is estimated as a

diagonal matrix, or as a full matrix. Default is TRUE (diagonal variance).

verbose logical flag indicating whether partition info is written in the console at each

MCMC iteration.

.. additional arguments to be passed to plot\_DPM. Only used if doPlot is TRUE.

#### Value

a object of class DPMclust with the following attributes:

mcmc\_partitions:

a list of length N. Each element mcmc\_partitions[n] is a vector of length n

giving the partition of the n observations.

alpha: a vector of length N. cost[j] is the cost associated to partition c[[j]]

U\_SS\_list: a list of length N containing the lists of sufficient statistics for all the mixture

components at each MCMC iteration

weights\_list: a list of length N containing the weights of each mixture component for each

MCMC iterations

logposterior\_list:

a list of length N containing the logposterior values at each MCMC iterations

data: the data matrix d x n with d dimensions in rows and n observations in columns

nb\_mcmcit: the number of MCMC iterations

clust\_distrib: the parametric distribution of the mixture component - "skewt"

hyperG0: the prior on the cluster location

## Author(s)

Boris Hejblum

#### References

Hejblum BP, Alkhassim C, Gottardo R, Caron F and Thiebaut R (2019) Sequential Dirichlet Process Mixtures of Multivariate Skew t-distributions for Model-based Clustering of Flow Cytometry Data. The Annals of Applied Statistics, 13(1): 638-660. <doi: 10.1214/18-AOAS1209> <arXiv: 1702.04407> https://arxiv.org/abs/1702.04407 doi:10.1214/18AOAS1209

```
rm(list=ls())
#Number of data
n <- 2000
set.seed(123)</pre>
```

```
d <- 2
ncl <- 4
# Sample data
sdev <- array(dim=c(d,d,ncl))</pre>
xi <- matrix(nrow=d, ncol=ncl, c(-1.5, 1, 1.5, 1, 1.5, -2, -2, -2))
psi <- matrix(nrow=d, ncol=4, c(0.4, -0.6, 0.8, 0, 0.3, -0.7, -0.3, -0.8))
nu <- c(100, 15, 8, 5)
p <- c(0.15, 0.05, 0.5, 0.3) # frequence des clusters
sdev[, ,1] \leftarrow matrix(nrow=d, ncol=d, c(0.3, 0, 0, 0.3))
sdev[, ,2] \leftarrow matrix(nrow=d, ncol=d, c(0.1, 0, 0, 0.3))
sdev[, ,3] <- matrix(nrow=d, ncol=d, c(0.3, 0.15, 0.15, 0.3))</pre>
sdev[, ,4] <- .3*diag(2)
c \leftarrow rep(0,n)
w \leftarrow rep(1,n)
z <- matrix(0, nrow=d, ncol=n)</pre>
for(k in 1:n){
c[k] = which(rmultinom(n=1, size=1, prob=p)!=0)
w[k] \leftarrow rgamma(1, shape=nu[c[k]]/2, rate=nu[c[k]]/2)
z[,k] \leftarrow xi[, c[k]] + psi[, c[k]]*rtruncnorm(n=1, a=0, b=Inf, mean=0, sd=1/sqrt(w[k])) +
            (sdev[, , c[k]]/sqrt(w[k]))**matrix(rnorm(d, mean = 0, sd = 1), nrow=d, ncol=1)
 \#cat(k, "/", n, " observations simulated\n", sep="")
# Set parameters of G0
hyperG0 <- list()</pre>
hyperG0[["b_xi"]] <- rowMeans(z)</pre>
hyperG0[["b_psi"]] \leftarrow rep(0,d)
hyperG0[["kappa"]] <- 0.001
hyperG0[["D_xi"]] <- 100
hyperG0[["D_psi"]] <- 100
hyperG0[["nu"]] <- d+1
hyperG0[["lambda"]] <- diag(apply(z,MARGIN=1, FUN=var))/3
 # hyperprior on the Scale parameter of DPM
 a <- 0.0001
 b <- 0.0001
 # do some plots
 nbclust_init <- 30</pre>
 ## Plot Data
 library(ggplot2)
 q <- (ggplot(data.frame("X"=z[1,], "Y"=z[2,]), aes(x=X, y=Y))</pre>
       + geom_point()
       + ggtitle("Simple example in 2d data")
       +xlab("D1")
       +ylab("D2")
       +theme_bw())
```

```
q
if(interactive()){
  MCMCsample_st <- DPMGibbsSkewT(z, hyperG0, a, b, N=2000,</pre>
                                                                                   doPlot=TRUE, plotevery=250,
                                                                                   nbclust_init, diagVar=FALSE,
                                                                                   gg.add=list(theme_bw(),
                                                               guides(shape=guide_legend(override.aes = list(fill="grey45")))))
   s <- summary(MCMCsample_st, burnin = 1500, thin=2, posterior_approx=TRUE)</pre>
  F <- FmeasureC(pred=s$point_estim$c_est, ref=c)</pre>
for(k in 1:n){
   c[k] = which(rmultinom(n=1, size=1, prob=p)!=0)
  w[k] \leftarrow rgamma(1, shape=nu[c[k]]/2, rate=nu[c[k]]/2)
  z[,k] \leftarrow xi[, c[k]] + psi[, c[k]]*rtruncnorm(n=1, a=0, b=Inf, mean=0, sd=1/sqrt(w[k])) + psi[, c[k]] + psi[, c[k]]*rtruncnorm(n=1, a=0, b=Inf, mean=0, sd=1/sqrt(w[k])) + psi[, c[k]] + psi[, c[k]]*rtruncnorm(n=1, a=0, b=Inf, mean=0, sd=1/sqrt(w[k])) + psi[, c[k]]*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w
                             (sdev[, , c[k]]/sqrt(w[k]))%*\\ %matrix(rnorm(d, mean = 0, sd = 1), nrow=d, ncol=1)
  cat(k, "/", n, " observations simulated\n", sep="")
}
   MCMCsample_st2 <- DPMGibbsSkewT_SeqPrior(z, prior=s$param_posterior,</pre>
                                                                                                            hyperG0, N=2000,
                                                                                                             doPlot=TRUE, plotevery=100,
                                                                                                            nbclust_init, diagVar=FALSE,
                                                                                                             gg.add=list(theme_bw(),
                                                               guides(shape=guide_legend(override.aes = list(fill="grey45")))))
s2 <- summary(MCMCsample_st2, burnin = 1500, thin=5)</pre>
F2 <- FmeasureC(pred=s2$point_estim$c_est, ref=c)
# MCMCsample_st2_par <- DPMGibbsSkewT_SeqPrior_parallel(Ncpus= 2, type_connec="SOCK",
                                                                                                                                           z, prior_inform=s$param_posterior,
#
                                                                                                                                                 hyperG0, N=2000,
#
                                                                                                                                                 doPlot=TRUE, plotevery=50,
                                                                                                                                                 nbclust_init, diagVar=FALSE,
                                                                                                                                                 gg.add=list(theme_bw(),
                                                                  guides(shape=guide_legend(override.aes = list(fill="grey45"))))
}
```

```
DPMGibbsSkewT_SeqPrior_parallel
```

Slice Sampling of Dirichlet Process Mixture of skew Student's t-distributions

#### **Description**

Slice Sampling of Dirichlet Process Mixture of skew Student's t-distributions

### Usage

```
DPMGibbsSkewT_SeqPrior_parallel(
```

```
Ncpus,
type_connec,
z,
prior_inform,
hyperG0,
N,
nbclust_init,
add.vagueprior = TRUE,
weightnoninfo = NULL,
doPlot = FALSE,
plotevery = N/10,
diagVar = TRUE,
verbose = TRUE,
monitorfile = "",
...
)
```

# Arguments

| Ncpus          | the number of processors available  |
|----------------|---|
| type_connec    | The type of connection between the processors. Supported cluster types are "SOCK", "FORK", "MPI", and "NWS". See also makeCluster.                                    |
| z              | data matrix d x n with d dimensions in rows and n observations in columns.  |
| prior_inform   | an informative prior such as the approximation computed by $\operatorname{summary}$ . $\operatorname{DPMMclust}$ .  |
| hyperG0        | prior mixing distribution.  |
| N              | number of MCMC iterations.  |
| nbclust_init   | number of clusters at initialization. Default to 30 (or less if there are less than 30 observations).   |
| add.vagueprior | logical flag indicating whether a non informative component should be added to the informative prior. Default is TRUE.  |
| weightnoninfo  | a real between 0 and 1 giving the weights of the non informative component in the prior.  |
| doPlot         | logical flag indicating whether to plot MCMC iteration or not. Default to TRUE.   |
| plotevery      | an integer indicating the interval between plotted iterations when doPlot is TRUE.  |
| diagVar        | logical flag indicating whether the variance of each cluster is estimated as a diagonal matrix, or as a full matrix. Default is TRUE (diagonal variance).             |
| verbose        | logical flag indicating whether partition info is written in the console at each MCMC iteration.  |
| monitorfile    | a writable connections or a character string naming a file to write into, to monitor the progress of the analysis. Default is "" which is no monitoring. See Details. |
|                | additional arguments to be passed to plot_DPM. Only used if doPlot is TRUE.   |

#### Value

a object of class DPMclust with the following attributes:

mcmc\_partitions:

a list of length N. Each element  $mcmc\_partitions[n]$  is a vector of length n

giving the partition of the n observations.

alpha: a vector of length N. cost[j] is the cost associated to partition c[[j]]

U\_SS\_list: a list of length N containing the lists of sufficient statistics for all the mixture

components at each MCMC iteration

weights\_list: a list of length N containing the logposterior values at each MCMC iterations

logposterior\_list:

a list of length N containing the logposterior values at each MCMC iterations

data: the data matrix d x n with d dimensions in rows and n observations in columns

nb\_mcmcit: the number of MCMC iterations

clust\_distrib: the parametric distribution of the mixture component - "skewt"

hyperG0: the prior on the cluster location

#### Author(s)

Boris Heiblum

#### References

Hejblum BP, Alkhassim C, Gottardo R, Caron F and Thiebaut R (2019) Sequential Dirichlet Process Mixtures of Multivariate Skew t-distributions for Model-based Clustering of Flow Cytometry Data. The Annals of Applied Statistics, 13(1): 638-660. <doi: 10.1214/18-AOAS1209> <arXiv: 1702.04407> https://arxiv.org/abs/1702.04407 doi:10.1214/18AOAS1209

```
rm(list=ls())
#Number of data
n <- 2000
set.seed(123)

d <- 2
ncl <- 4

# Sample data

sdev <- array(dim=c(d,d,ncl))

#xi <- matrix(nrow=d, ncol=ncl, c(-1.5, 1.5, 1.5, 1.5, 2, -2.5, -2.5, -3))
#psi <- matrix(nrow=d, ncol=4, c(0.4, -0.6, 0.8, 0, 0.3, -0.7, -0.3, -0.8))
xi <- matrix(nrow=d, ncol=ncl, c(-0.2, 0.5, 2.4, 0.4, 0.6, -1.3, -0.9, -2.7))
psi <- matrix(nrow=d, ncol=4, c(0.3, -0.7, -0.8, 0, 0.3, -0.7, 0.2, 0.9))</pre>
```

```
nu <- c(100, 15, 8, 5)
p <- c(0.15, 0.05, 0.5, 0.3) # frequence des clusters
sdev[, ,1] \leftarrow matrix(nrow=d, ncol=d, c(0.3, 0, 0, 0.3))
sdev[, ,2] \leftarrow matrix(nrow=d, ncol=d, c(0.1, 0, 0, 0.3))
sdev[, ,3] <- matrix(nrow=d, ncol=d, c(0.3, 0.15, 0.15, 0.3))</pre>
sdev[, ,4] <- .3*diag(2)</pre>
c \leftarrow rep(0,n)
w <- rep(1,n)
z <- matrix(0, nrow=d, ncol=n)</pre>
for(k in 1:n){
  c[k] = which(rmultinom(n=1, size=1, prob=p)!=0)
  w[k] \leftarrow rgamma(1, shape=nu[c[k]]/2, rate=nu[c[k]]/2)
  z[,k] \leftarrow xi[, c[k]] + psi[, c[k]]*rtruncnorm(n=1, a=0, b=Inf, mean=0, sd=1/sqrt(w[k])) + psi[, c[k]] + psi[, c[k]]*rtruncnorm(n=1, a=0, b=Inf, mean=0, sd=1/sqrt(w[k])) + psi[, c[k]] + psi[, c[k]]*rtruncnorm(n=1, a=0, b=Inf, mean=0, sd=1/sqrt(w[k])) + psi[, c[k]]*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w[k])*rtruncnorm(w
                           (sdev[, , c[k]]/sqrt(w[k])) %* matrix(rnorm(d, mean = 0, sd = 1), nrow=d, ncol=1)
  \#cat(k, "/", n, " observations simulated\n", sep="")
}
# Set parameters of G0
hyperG0 <- list()</pre>
hyperG0[["b_xi"]] <- rowMeans(z)</pre>
hyperG0[["b_psi"]] <- rep(0,d)
hyperG0[["kappa"]] <- 0.001
hyperG0[["D_xi"]] <- 100
hyperG0[["D_psi"]] <- 100
hyperG0[["nu"]] <- d+1
hyperG0[["lambda"]] <- diag(apply(z,MARGIN=1, FUN=var))/3
  # hyperprior on the Scale parameter of DPM
  a <- 0.0001
  b <- 0.0001
  # do some plots
  nbclust_init <- 30</pre>
  ## Plot Data
  library(ggplot2)
  q \leftarrow (ggplot(data.frame("X"=z[1,], "Y"=z[2,]), aes(x=X, y=Y))
                 + geom_point()
                 + ggtitle("Simple example in 2d data")
                 +xlab("D1")
                 +ylab("D2")
                 +theme_bw())
if(interactive()){
  MCMCsample_st <- DPMGibbsSkewT(z, hyperG0, a, b, N=2000,</pre>
                                                                              doPlot=TRUE, plotevery=250,
                                                                              nbclust_init,
                                                                               gg.add=list(theme_bw(),
                                                            guides(shape=guide_legend(override.aes = list(fill="grey45")))),
                                                                              diagVar=FALSE)
```

```
s <- summary(MCMCsample_st, burnin = 1500, thin=5, posterior_approx=TRUE)
 F <- FmeasureC(pred=s$point_estim$c_est, ref=c)</pre>
for(k in 1:n){
 c[k] = which(rmultinom(n=1, size=1, prob=p)!=0)
 w[k] \leftarrow rgamma(1, shape=nu[c[k]]/2, rate=nu[c[k]]/2)
 z[,k] \leftarrow xi[, c[k]] + psi[, c[k]]*rtruncnorm(n=1, a=0, b=Inf, mean=0, sd=1/sqrt(w[k])) +
           (sdev[, , c[k]]/sqrt(w[k]))%*\\ %matrix(rnorm(d, mean = 0, sd = 1), nrow=d, ncol=1)
 \#cat(k, "/", n, " observations simulated\n", sep="")
}
MCMCsample_st2 <- DPMGibbsSkewT_SeqPrior_parallel(Ncpus=2, type_connec="SOCK",
                                                     z, prior_inform=s$param_posterior,
                                                    hyperG0, N=3000,
                                                     doPlot=TRUE, plotevery=100,
                                               nbclust_init, diagVar=FALSE, verbose=FALSE,
                                                    gg.add=list(theme_bw(),
                         guides(shape=guide_legend(override.aes = list(fill="grey45")))))
s2 <- summary(MCMCsample_st2, burnin = 2000, thin=5)</pre>
F2 <- FmeasureC(pred=s2$point_estim$c_est, ref=c)
}
```

DPMpost

Posterior estimation for Dirichlet process mixture of multivariate (potentially skew) distributions models

## **Description**

Partially collapse slice Gibbs sampling for Dirichlet process mixture of multivariate normal, skew normal or skew t distributions.

## Usage

```
DPMpost(
  data,
  hyperG0,
  a = 1e-04,
  b = 1e-04,
  N,
  doPlot = TRUE,
  nbclust_init = 30,
  plotevery = floor(N/10),
  diagVar = TRUE,
  verbose = TRUE,
  distrib = c("gaussian", "skewnorm", "skewt"),
  ncores = 1,
  type_connec = "SOCK",
  informPrior = NULL,
```

)

#### **Arguments**

data data matrix d x n with d dimensions in rows and n observations in columns. hyperG0 prior mixing distribution. shape hyperparameter of the Gamma prior on the concentration parameter of the а Dirichlet Process. Default is 0.0001. b scale hyperparameter of the Gamma prior on the concentration parameter of the Dirichlet Process. Default is 0.0001. If 0, then the concentration is fixed set to Ν number of MCMC iterations. doPlot logical flag indicating whether to plot MCMC iteration or not. Default to TRUE. nbclust\_init number of clusters at initialization. Default to 30 (or less if there are less than 30 observations). an integer indicating the interval between plotted iterations when doPlot is plotevery TRUE. logical flag indicating whether the variance of each cluster is estimated as a diagVar diagonal matrix, or as a full matrix. Default is TRUE (diagonal variance). verbose logical flag indicating whether partition info is written in the console at each MCMC iteration. distrib the distribution used for the clustering. Current possibilities are "gaussian", "skewnorm" and "skewt". number of cores to use. ncores The type of connection between the processors. Supported cluster types are type\_connec

"SOCK", "FORK", "MPI", and "NWS". See also makeCluster.

## **Details**

informPrior

This function is a wrapper around the following functions: DPMGibbsN, DPMGibbsN\_parallel, DPMGibbsN\_SeqPrior, DPMGibbsSkewN, DPMGibbsSkewN\_parallel, DPMGibbsSkewT, DPMGibbsSkewT\_parallel, DPMGibbsSkewT\_SeqPrior, DPMGibbsSkewT\_seqPrior\_parallel.

additional arguments to be passed to plot\_DPM. Only used if doPlot is TRUE.

an optional informative prior such as the approximation computed by summary. DPMMclust.

#### Value

a object of class DPMclust with the following attributes:

mcmc\_partitions:

a list of length N. Each element  $mcmc\_partitions[n]$  is a vector of length n

giving the partition of the n observations.

alpha: a vector of length N. cost[j] is the cost associated to partition c[[j]]

U\_SS\_list: a list of length N containing the lists of sufficient statistics for all the mixture

components at each MCMC iteration

weights\_list: a list of length N containing the weights of each mixture component for each

MCMC iterations

logposterior\_list:

a list of length N containing the logposterior values at each MCMC iterations

data: the data matrix d x n with d dimensions in rows and n observations in columns

nb\_mcmcit: the number of MCMC iterations

clust\_distrib: the parametric distribution of the mixture component

hyperG0: the prior on the cluster location

### Author(s)

Boris Hejblum

#### References

Hejblum BP, Alkhassim C, Gottardo R, Caron F and Thiebaut R (2019) Sequential Dirichlet Process Mixtures of Multivariate Skew t-distributions for Model-based Clustering of Flow Cytometry Data. The Annals of Applied Statistics, 13(1): 638-660. <doi: 10.1214/18-AOAS1209> <arXiv: 1702.04407> https://arxiv.org/abs/1702.04407 doi:10.1214/18AOAS1209

#### See Also

```
summary.DPMMclust
```

```
#rm(list=ls())
set.seed(123)
# Exemple in 2 dimensions with skew-t distributions
# Generate data:
n <- 2000 # number of data points
d <- 2 # dimensions
ncl <- 4 # number of true clusters
sdev <- array(dim=c(d,d,ncl))</pre>
xi <- matrix(nrow=d, ncol=ncl, c(-1.5, 1.5, 1.5, 1.5, 2, -2.5, -2.5, -3))
psi <- matrix(nrow=d, ncol=4, c(0.3, -0.7, -0.8, 0, 0.3, -0.7, 0.2, 0.9))
nu <- c(100, 25, 8, 5)
proba <- c(0.15, 0.05, 0.5, 0.3) # cluster frequencies
sdev[, ,1] \leftarrow matrix(nrow=d, ncol=d, c(0.3, 0, 0, 0.3))
sdev[, ,2] \leftarrow matrix(nrow=d, ncol=d, c(0.1, 0, 0, 0.3))
sdev[, ,3] \leftarrow matrix(nrow=d, ncol=d, c(0.3, 0, 0, 0.2))
sdev[, ,4] <- .3*diag(2)
c \leftarrow rep(0,n)
w <- rep(1,n)
z <- matrix(0, nrow=d, ncol=n)</pre>
for(k in 1:n){
```

```
c[k] = which(rmultinom(n=1, size=1, prob=proba)!=0)
w[k] \leftarrow rgamma(1, shape=nu[c[k]]/2, rate=nu[c[k]]/2)
z[,k] \leftarrow xi[, c[k]] + psi[, c[k]]*rtruncnorm(n=1, a=0, b=Inf, mean=0, sd=1/sqrt(w[k])) +
           (sdev[, , c[k]]/sqrt(w[k]))%*%matrix(rnorm(d, mean = 0, sd = 1), nrow=d, ncol=1)
}
# Define hyperprior
hyperG0 <- list()</pre>
hyperG0[["b_xi"]] <- rowMeans(z)</pre>
hyperG0[["b_psi"]] <- rep(0,d)
hyperG0[["kappa"]] <- 0.001
hyperG0[["D_xi"]] <- 100
hyperG0[["D_psi"]] <- 100
hyperG0[["nu"]] <- d+1
hyperG0[["lambda"]] <- diag(apply(z,MARGIN=1, FUN=var))/3</pre>
if(interactive()){
# Plot data
cytoScatter(z)
# Estimate posterior
MCMCsample_st <- DPMpost(data=z, hyperG0=hyperG0, N=2000,</pre>
   distrib="skewt",
   gg.add=list(ggplot2::theme_bw(),
      ggplot2::guides(shape=ggplot2::guide_legend(override.aes = list(fill="grey45"))))
 s <- summary(MCMCsample_st, burnin = 1600, thin=5, lossFn = "Binder")</pre>
plot(s)
 #plot(s, hm=TRUE) # this can take a few sec...
 # more data plotting:
 library(ggplot2)
 p \leftarrow (ggplot(data.frame("X"=z[1,], "Y"=z[2,]), aes(x=X, y=Y))
       + geom_point()
       + ggtitle("Unsupervised data")
       + xlab("D1")
       + ylab("D2")
       + theme_bw()
)
р
c2plot <- factor(c)</pre>
 levels(c2plot) <- c("4", "1", "3", "2")
 pp <- (ggplot(data.frame("X"=z[1,], "Y"=z[2,], "Cluster"=as.character(c2plot)))</pre>
       + geom_point(aes(x=X, y=Y, colour=Cluster, fill=Cluster))
       + ggtitle("True clusters")
       + xlab("D1")
       + ylab("D2")
       + theme_bw()
     + scale_colour_discrete(guide=guide_legend(override.aes = list(size = 6, shape=22)))
```

```
)
 pp
}
# Exemple in 2 dimensions with Gaussian distributions
set.seed(1234)
# Generate data
n <- 2000 # number of data points
d <- 2 # dimensions
ncl <- 4 # number of true clusters
m \leftarrow matrix(nrow=2, ncol=4, c(-1, 1, 1.5, 2, 2, -2, -1.5, -2)) # cluster means
sdev <- array(dim=c(2, 2, 4)) # cluster standard-deviations</pre>
sdev[, ,1] \leftarrow matrix(nrow=2, ncol=2, c(0.3, 0, 0, 0.3))
sdev[, ,2] \leftarrow matrix(nrow=2, ncol=2, c(0.1, 0, 0, 0.3))
sdev[, ,3] <- matrix(nrow=2, ncol=2, c(0.3, 0.15, 0.15, 0.3))</pre>
sdev[, ,4] <- .3*diag(2)
proba <- c(0.15, 0.05, 0.5, 0.3) # cluster frequencies
c \leftarrow rep(0,n)
z <- matrix(0, nrow=2, ncol=n)</pre>
for(k in 1:n){
c[k] = which(rmultinom(n=1, size=1, prob=proba)!=0)
z[,k] \leftarrow m[, c[k]] + sdev[, , c[k]]**matrix(rnorm(2, mean = 0, sd = 1), nrow=2, ncol=1)
# Define hyperprior
hyperG0 <- list()</pre>
hyperG0[["mu"]] <- rep(0,d)
hyperG0[["kappa"]] <- 0.001
hyperG0[["nu"]] <- d+2
hyperG0[["lambda"]] <- diag(d)</pre>
if(interactive()){
# Plot data
cytoScatter(z)
# Estimate posterior
MCMCsample_n <- DPMpost(data=z, hyperG0=hyperG0, N=2000,</pre>
   distrib="gaussian", diagVar=FALSE,
   gg.add=list(ggplot2::theme_bw(),
      ggplot2::guides(shape=ggplot2::guide_legend(override.aes = list(fill="grey45"))))
 s <- summary(MCMCsample_n, burnin = 1500, thin=5, lossFn = "Binder")</pre>
 s
 plot(s)
 #plot(s, hm=TRUE) # this can take a few sec...
```

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```
# more data plotting:
library(ggplot2)
p \leftarrow (ggplot(data.frame("X"=z[1,], "Y"=z[2,]), aes(x=X, y=Y))
       + geom_point()
       + ggtitle("Unsupervised data")
       + xlab("D1")
       + ylab("D2")
       + theme_bw()
)
р
c2plot <- factor(c)</pre>
levels(c2plot) <- c("4", "1", "3", "2")
pp <- (ggplot(data.frame("X"=z[1,], "Y"=z[2,], "Cluster"=as.character(c2plot)))</pre>
       + geom_point(aes(x=X, y=Y, colour=Cluster, fill=Cluster))
       #+ ggtitle("Slightly overlapping skew-normal simulation\n")
       + xlab("D1")
       + ylab("D2")
       + theme_bw()
     + scale_colour_discrete(guide=guide_legend(override.aes = list(size = 6, shape=22)))
       + ggtitle("True clusters")
)
pp
}
```

evalClustLoss

ELoss of a partition point estimate compared to a gold standard

## **Description**

Evaluate the loss of a point estimate of the partition compared to a gold standard according to a given loss function

## Usage

```
evalClustLoss(c, gs, lossFn = "F-measure", a = 1, b = 1)
```

## **Arguments**

| gs vector of length n containing the gold standard partition of the n observables.  lossFn character string specifying the loss function to be used. Either "F-me" "Binder" (see Details). Default is "F-measure".  a only relevant if lossFn is "Binder". Penalty for wrong co-clustering pared to gs. Defaults is 1. |            |
|--|------------|
| "Binder" (see Details). Default is "F-measure".  a only relevant if lossFn is "Binder". Penalty for wrong co-clustering  |            |
|  | easure" or |
|  | in c com-  |
| b only relevant if lossFn is "Binder". Penalty for missed co-clustering pared to gs. Defaults is 1.  | in c com-  |

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#### **Details**

The cost of a point estimate partition is calculated using either a pairwise coincidence loss function (Binder), or 1-Fmeasure (F-measure).

#### Value

the cost of the point estimate c in regard of the gold standard gs for a given loss function.

#### Author(s)

Boris Hejblum

#### References

J.W. Lau & P.J. Green. Bayesian Model-Based Clustering Procedures, Journal of Computational and Graphical Statistics, 16(3): 526-558, 2007.

D. B. Dahl. Model-Based Clustering for Expression Data via a Dirichlet Process Mixture Model, in Bayesian Inference for Gene Expression and Proteomics, K.-A. Do, P. Muller, M. Vannucci (Eds.), Cambridge University Press, 2006.

#### See Also

```
similarityMat, cluster_est_binder
```

Flimited

Compute a limited F-measure

#### **Description**

A limited version of F-measure that only takes into account small clusters

#### Usage

```
Flimited(n_small_clst, pred, ref)
```

#### Arguments

n\_small\_clst an integer for limit size of the small cluster

pred vector of a predicted partition
ref vector of a reference partition

#### References

Hejblum BP, Alkhassim C, Gottardo R, Caron F and Thiebaut R (2019) Sequential Dirichlet Process Mixtures of Multivariate Skew t-distributions for Model-based Clustering of Flow Cytometry Data. The Annals of Applied Statistics, 13(1): 638-660. <doi: 10.1214/18-AOAS1209> <arXiv: 1702.04407> https://arxiv.org/abs/1702.04407 doi:10.1214/18AOAS1209

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## **Examples**

```
pred <- c(rep(1, 5),rep(2, 8),rep(3,10))
ref <- c(rep(1, 5),rep(c(2,3), 4),rep(c(3,2),5))
FmeasureC(pred, ref)
Flimited(6, pred, ref)</pre>
```

FmeasureC

*C++ implementation of the F-measure computation* 

## **Description**

C++ implementation of the F-measure computation

## Usage

```
FmeasureC(pred, ref)
```

# Arguments

pred vector of a predicted partition ref vector of a reference partition

## **Examples**

```
pred <- c(1,1,2,3,2,3)
ref <- c(2,2,1,1,1,3)
FmeasureC(pred, ref)</pre>
```

FmeasureC\_no0

C++ implementation of the F-measure computation without the reference class 0

# Description

Aghaeepour in FlowCAP 1 ignore the reference class labeled "0"

#### Usage

```
FmeasureC_no0(pred, ref)
```

## Arguments

pred vector of a predicted partition ref vector of a reference partition 56 Fmeasure\_costC

#### References

N Aghaeepour, G Finak, H Hoos, TR Mosmann, RR Brinkman, R Gottardo, RH Scheuermann, Critical assessment of automated flow cytometry data analysis techniques, *Nature Methods*, 10(3):228-38, 2013.

## **Examples**

```
library(NPflow)
pred <- c(1,1,2,3,2,3)
ref <- c(2,2,0,0,0,3)
FmeasureC(pred, ref)
FmeasureC_no0(pred, ref)</pre>
```

Fmeasure\_costC

Multiple cost computations with the F-measure as the loss function

## Description

C++ implementation of multiple cost computations with the F-measure as the loss function using the Armadillo library

## Usage

```
Fmeasure_costC(c)
```

## **Arguments**

С

a matrix where each column is one MCMC partition

#### Value

a list with the following elements:

Fmeas: TODO cost: TODO

```
library(NPflow)
c <- list(c(1,1,2,3,2,3), c(1,1,1,2,3,3),c(2,2,1,1,1,1))
#Fmeasure_costC(sapply(c, "["))

if(interactive()){
   c2 <- list()
   for(i in 1:100){
      c2 <- c(c2, list(rmultinom(n=1, size=2000, prob=rexp(n=2000))))
}
Fmeasure_costC(sapply(c2, "["))</pre>
```

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}

lgamma\_mv

Multivariate log gamma function

# Description

Multivariate log gamma function

## Usage

```
lgamma_mv(x, p)
```

# Arguments

x strictly positive real number

p integer

MAP\_sNiW\_mmEM

EM MAP for mixture of sNiW

# Description

Maximum A Posteriori (MAP) estimation of mixture of Normal inverse Wishart distributed observations with an EM algorithm

## Usage

```
MAP_sNiW_mmEM(
    xi_list,
    psi_list,
    S_list,
    hyperG0,
    init = NULL,
    K,
    maxit = 100,
    tol = 0.1,
    doPlot = TRUE,
    verbose = TRUE
)

MAP_sNiW_mmEM_weighted(
    xi_list,
    psi_list,
```

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```
S_list,
  obsweight_list,
  hyperG0,
  Κ,
  maxit = 100,
  tol = 0.1,
  doPlot = TRUE,
  verbose = TRUE
)
MAP_sNiW_mmEM_vague(
  xi_list,
  psi_list,
  S_list,
  hyperG0,
  K = 10,
  maxit = 100,
  tol = 0.1,
  doPlot = TRUE,
  verbose = TRUE
)
```

## **Arguments**

| xi_list        | a list of length n, each element is a vector of size d containing the argument xi of the corresponding allocated cluster.   |
|----------------|---|
| psi_list       | a list of length n, each element is a vector of size d containing the argument psi of the corresponding allocated cluster.  |
| S_list         | a list of length $n$ , each element is a matrix of size $d \times d$ containing the argument $S$ of the corresponding allocated cluster.                                    |
| hyperG0        | prior mixing distribution used if init is NULL.   |
| init           | a list for initializing the algorithm with the following elements: b_xi, b_psi, lambda, B, nu. Default is NULL in which case the initialization of the algorithm is random. |
| K              | integer giving the number of mixture components.  |
| maxit          | integer giving the maximum number of iteration for the EM algorithm. Default is 100.  |
| tol            | real number giving the tolerance for the stopping of the EM algorithm. Default is $\emptyset.1$ .   |
| doPlot         | a logical flag indicating whether the algorithm progression should be plotted. Default is TRUE.   |
| verbose        | logical flag indicating whether plot should be drawn. Default is TRUE.  |
| obsweight_list | a list of length n where each element is a vector of weights for each sampled cluster at each MCMC iterations.  |

MAP\_sNiW\_mmEM

# **Details**

MAP\_sNiW\_mmEM provides an estimation for the MAP of mixtures of Normal inverse Wishart distributed observations. MAP\_sNiW\_mmEM\_vague provides an estimates incorporating a vague component in the mixture. MAP\_sNiW\_mmEM\_weighted provides a weighted version of the algorithm.

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## Author(s)

Boris Hejblum, Chariff Alkhassim

```
set.seed(1234)
hyperG0 <- list()</pre>
hyperG0$b_xi <- c(0.3, -1.5)
hyperG0$b_psi <- c(0, 0)
hyperG0$kappa <- 0.001
hyperG0$D_xi <- 100
hyperG0$D_psi <- 100
hyperG0$nu <- 20
hyperG0$lambda <- diag(c(0.25,0.35))
hyperG0 <- list()</pre>
hyperG0$b_xi <- c(1, -1.5)
hyperG0$b_psi <- c(0, 0)
hyperG0$kappa <- 0.1
hyperG0$D_xi <- 1
hyperG0$D_psi <- 1
hyperG0$nu <- 2
hyperG0$lambda <- diag(c(0.25,0.35))
xi_list <- list()</pre>
psi_list <- list()</pre>
S_list <- list()</pre>
w_list <- list()</pre>
for(k in 1:200){
 NNiW <- rNNiW(hyperG0, diagVar=FALSE)
 xi_list[[k]] <- NNiW[["xi"]]</pre>
 psi_list[[k]] <- NNiW[["psi"]]</pre>
 S_list[[k]] <- NNiW[["S"]]</pre>
 w_{list}[[k]] < 0.75
}
hyperG02 <- list()</pre>
hyperG02b_xi < c(-1, 2)
hyperG02b_psi < c(-0.1, 0.5)
hyperG02$kappa <- 0.1
hyperG02$D_xi <- 1
hyperG02$D_psi <- 1
hyperG02$nu <- 4
hyperG02$lambda <- 0.5*diag(2)</pre>
```

MLE\_gamma

```
for(k in 201:400){
  NNiW <- rNNiW(hyperG02, diagVar=FALSE)
  xi_list[[k]] <- NNiW[["xi"]]
  psi_list[[k]] <- NNiW[["psi"]]
  S_list[[k]] <- NNiW[["S"]]
  w_list [[k]] <- 0.25
}
map <- MAP_sNiW_mmEM(xi_list, psi_list, S_list, hyperG0, K=2, tol=0.1)</pre>
```

MLE\_gamma

MLE for Gamma distribution

## **Description**

Maximum likelihood estimation of Gamma distributed observations distribution parameters

# Usage

```
MLE_gamma(g)
```

## **Arguments**

g

a list of Gamma distributed observation.

```
g_list <- list()
for(i in 1:1000){
   g_list <- c(g_list, rgamma(1, shape=100, rate=5))
}
mle <- MLE_gamma(g_list)
mle</pre>
```

MLE\_NiW\_mmEM 61

 ${\sf MLE\_NiW\_mmEM}$ 

EM MLE for mixture of NiW

# Description

Maximum likelihood estimation of mixture of Normal inverse Wishart distributed observations with an EM algorithm

# Usage

```
MLE_NiW_mmEM(
   mu_list,
   S_list,
   hyperG0,
   K,
   maxit = 100,
   tol = 0.1,
   doPlot = TRUE
)
```

# Arguments

| mu_list | a list of length N whose elements are observed vectors of length d of the mean parameters.                     |
|---------|--|
| S_list  | a list of length N whose elements are observed variance-covariance matrices of dimension d $\boldsymbol{x}$ d. |
| hyperG0 | prior mixing distribution used for randomly initializing the algorithm.  |
| K       | integer giving the number of mixture components.   |
| maxit   | integer giving the maximum number of iteration for the EM algorithm. Default is 100.                           |
| tol     | real number giving the tolerance for the stopping of the EM algorithm. Default is $\emptyset.1$ .              |
| doPlot  | a logical flag indicating whether the algorithm progression should be plotted. Default is TRUE.                |

```
set.seed(123)
U_mu <- list()
U_Sigma <- list()
U_nu<-list()
U_kappa<-list()

d <- 2
hyperG0 <- list()
hyperG0[["mu"]] <- rep(1,d)</pre>
```

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```
hyperG0[["kappa"]] <- 0.01
hyperG0[["nu"]] <- d+1
hyperG0[["lambda"]] <- diag(d)</pre>
for(k in 1:200){
  NiW <- rNiW(hyperG0, diagVar=FALSE)
  U_mu[[k]] <-NiW[["mu"]]
  U_Sigma[[k]] <-NiW[["S"]]
}
hyperG02 <- list()</pre>
hyperG02[["mu"]] <- rep(2,d)
hyperG02[["kappa"]] <- 1</pre>
hyperG02[["nu"]] <- d+10
hyperG02[["lambda"]] \leftarrow diag(d)/10
for(k in 201:400){
  NiW <- rNiW(hyperG02, diagVar=FALSE)
  U_mu[[k]] <-NiW[["mu"]]</pre>
  U_Sigma[[k]] <-NiW[["S"]]
}
mle <- MLE_NiW_mmEM( U_mu, U_Sigma, hyperG0, K=2)</pre>
hyperG0[["mu"]]
hyperG02[["mu"]]
mle$U_mu
hyperG0[["lambda"]]
hyperG02[["lambda"]]
mle$U_lambda
hyperG0[["nu"]]
hyperG02[["nu"]]
mle$U_nu
hyperG0[["kappa"]]
hyperG02[["kappa"]]
mle$U_kappa
```

MLE\_sNiW

MLE for sNiW distributed observations

## **Description**

Maximum likelihood estimation of Normal inverse Wishart distributed observations

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#### Usage

```
MLE_sNiW(xi_list, psi_list, S_list, doPlot = TRUE)
```

## **Arguments**

| xi_list  | a list of length N whose elements are observed vectors of length d of the mean parameters xi.                  |
|----------|--|
| psi_list | a list of length N whose elements are observed vectors of length d of the skew parameters psi.                 |
| S_list   | a list of length N whose elements are observed variance-covariance matrices of dimension d $\boldsymbol{x}$ d. |
| doPlot   | a logical flag indicating whether the algorithm progression should be plotted. Default is TRUE.                |

## Author(s)

Boris Hejblum, Chariff Alkhassim

## **Examples**

```
hyperG0 <- list()</pre>
hyperG0$b_xi <- c(0.3, -1.5)
hyperG0$b_psi <- c(0, 0)
hyperG0$kappa <- 0.001
hyperG0$D_xi <- 100
hyperG0$D_psi <- 100</pre>
hyperG0$nu <- 35
hyperG0\$lambda <- diag(c(0.25,0.35))
xi_list <- list()</pre>
psi_list <- list()</pre>
S_list <- list()</pre>
for(k in 1:1000){
NNiW <- rNNiW(hyperG0, diagVar=FALSE)</pre>
 xi_list[[k]] <- NNiW[["xi"]]</pre>
 psi_list[[k]] <- NNiW[["psi"]]</pre>
 S_list[[k]] <- NNiW[["S"]]</pre>
}
mle <- MLE_sNiW(xi_list, psi_list, S_list)</pre>
mle
```

MLE\_sNiW\_mmEM

EM MLE for mixture of sNiW

#### **Description**

Maximum likelihood estimation of mixture of Normal inverse Wishart distributed observations with an EM algorithm

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# Usage

```
MLE_sNiW_mmEM(
    xi_list,
    psi_list,
    S_list,
    hyperG0,
    K,
    init = NULL,
    maxit = 100,
    tol = 0.1,
    doPlot = TRUE,
    verbose = TRUE
)
```

# Arguments

| xi_list  | a list of length N whose elements are observed vectors of length d of the mean parameters $xi$ .  |
|----------|---|
| psi_list | a list of length N whose elements are observed vectors of length d of the skew parameters psi.  |
| S_list   | a list of length N whose elements are observed variance-covariance matrices of dimension d $\boldsymbol{x}$ d.  |
| hyperG0  | prior mixing distribution used if init is NULL.   |
| K        | integer giving the number of mixture components.  |
| init     | a list for initializing the algorithm with the following elements: b_xi, b_psi, lambda, B, nu. Default is NULL in which case the initialization of the algorithm is random. |
| maxit    | integer giving the maximum number of iteration for the EM algorithm. Default is 100.  |
| tol      | real number giving the tolerance for the stopping of the EM algorithm. Default is $\emptyset.1$ .   |
| doPlot   | a logical flag indicating whether the algorithm progression should be plotted. Default is TRUE.   |
| verbose  | logical flag indicating whether plot should be drawn. Default is TRUE.  |

# Author(s)

Boris Hejblum, Chariff Alkhassim

```
set.seed(1234)
hyperG0 <- list()
hyperG0$b_xi <- c(0.3, -1.5)
hyperG0$b_psi <- c(0, 0)
hyperG0$kappa <- 0.001</pre>
```

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```
hyperG0$D_xi <- 100
hyperG0$D_psi <- 100
hyperG0$nu <- 3
hyperG0\$lambda <- diag(c(0.25,0.35))
xi_list <- list()</pre>
psi_list <- list()</pre>
S_list <- list()</pre>
for(k in 1:200){
 NNiW <- rNNiW(hyperG0, diagVar=FALSE)
 xi_list[[k]] <- NNiW[["xi"]]</pre>
 psi_list[[k]] <- NNiW[["psi"]]</pre>
 S_list[[k]] <- NNiW[["S"]]</pre>
hyperG02 <- list()</pre>
hyperG02b_xi < c(-1, 2)
hyperG02b_psi < c(-0.1, 0.5)
hyperG02$kappa <- 0.001
hyperG02$D_xi <- 10
hyperG02$D_psi <- 10
hyperG02$nu <- 3
hyperG02$lambda <- 0.5*diag(2)</pre>
for(k in 201:400){
NNiW <- rNNiW(hyperG02, diagVar=FALSE)</pre>
 xi_list[[k]] <- NNiW[["xi"]]</pre>
 psi_list[[k]] <- NNiW[["psi"]]</pre>
 S_list[[k]] <- NNiW[["S"]]</pre>
}
mle <- MLE_sNiW_mmEM(xi_list, psi_list, S_list, hyperG0, K=2)</pre>
```

mmNiWpdf

multivariate Normal inverse Wishart probability density function for multiple inputs

## **Description**

multivariate Normal inverse Wishart probability density function for multiple inputs

#### Usage

```
mmNiWpdf(mu, Sigma, U_mu0, U_kappa0, U_nu0, U_lambda0, Log = TRUE)
```

#### **Arguments**

mu

data matrix of dimension  $p \times n$ , p being the dimension of the data and n the number of data points, where each column is an observed mean vector.

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| Sigma     | list of length n of observed variance-covariance matrices, each of dimensions $p \times p$ .  |
|-----------|---|
| U_mu0     | mean vectors matrix of dimension $p \times K$ , $K$ being the number of distributions for which the density probability has to be evaluated |
| U_kappa0  | vector of length K of scale parameters.   |
| U_nu0     | vector of length K of degree of freedom parameters.   |
| U_lambda0 | list of length K of variance-covariance matrices, each of dimensions p x p.   |
| Log       | logical flag for returning the log of the probability density function. Defaults is TRUE.   |

# Value

matrix of densities of dimension K x n

| · | C++ implementation of multivariate Normal inverse Wishart proba-<br>ility density function for multiple inputs |
|---|--|
|---|--|

# Description

C++ implementation of multivariate Normal inverse Wishart probability density function for multiple inputs

# Usage

```
mmNiWpdfC(Mu, Sigma, U_Mu0, U_Kappa0, U_Nu0, U_Sigma0, Log = TRUE)
```

# Arguments

| Mu       | data matrix of dimension $p \times n$ , $p$ being the dimension of the data and $n$ the number of data points, where each column is an observed mean vector. |
|----------|--|
| Sigma    | list of length n of observed variance-covariance matrices, each of dimensions p ${\sf x}$ p.   |
| U_Mu0    | mean vectors matrix of dimension $p \times K$ , $K$ being the number of distributions for which the density probability has to be evaluated                  |
| U_Kappa0 | vector of length K of scale parameters.  |
| U_Nu0    | vector of length K of degree of freedom parameters.  |
| U_Sigma0 | list of length K of variance-covariance matrices, each of dimensions p x p.  |
| Log      | logical flag for returning the log of the probability density function. Defaults is TRUE.  |

# Value

matrix of densities of dimension K x n

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#### References

Hejblum BP, Alkhassim C, Gottardo R, Caron F and Thiebaut R (2019) Sequential Dirichlet Process Mixtures of Multivariate Skew t-distributions for Model-based Clustering of Flow Cytometry Data. The Annals of Applied Statistics, 13(1): 638-660. <doi: 10.1214/18-AOAS1209>. <arXiv: 1702.04407>. https://arxiv.org/abs/1702.04407 doi:10.1214/18AOAS1209

| Wishart | O1 | Probability density function of multiple structured Normal inverse<br>Wishart |
|---------|----|---|
|---------|----|---|

## **Description**

Probability density function of structured Normal inverse Wishart (sNiW) for multiple inputs, on the log scale.

## Usage

```
mmsNiWlogpdf(U_xi, U_psi, U_Sigma, U_xi0, U_psi0, U_B0, U_Sigma0, U_df0)
```

## **Arguments**

| U_xi     | a list of length n of observed mean vectors, each of dimension p                             |
|----------|--|
| U_psi    | a list of length n of observed skew vectors of dimension p                                   |
| U_Sigma  | a list of length n of observed covariance matrices, each of dimension p x p                  |
| U_xi0    | a list of length K of mean vector parameters for sNiW, each of dimension p                   |
| U_psi0   | a list of length K of mean vector parameters for sNiW, each of dimension p                   |
| U_B0     | a list of length K of structuring matrix parameters for sNiW, each of dimension $2 \times 2$ |
| U_Sigma0 | a list of length K of covariance matrix parameters for sNiW, each of dimension $p \ x \ p$   |
| U_df0    | a list of length K of degrees of freedom parameters for sNiW, each of dimension p x p $$     |

```
hyperG0 <- list()
hyperG0$b_xi <- c(-1.6983129, -0.4819131)
hyperG0$b_psi <- c(-0.0641866, -0.7606068)
hyperG0$kappa <- 0.001
hyperG0$D_xi <- 16.951313
hyperG0$D_psi <- 1.255192
hyperG0$nu <- 27.67656
hyperG0$lambda <- matrix(c(2.3397761, -0.3975259, -0.3975259, 1.9601773), ncol=2)

xi_list <- list()
psi_list <- list()</pre>
```

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```
S_list <- list()</pre>
for(k in 1:1000){
NNiW <- rNNiW(hyperG0, diagVar=FALSE)
xi_list[[k]] <- NNiW[["xi"]]</pre>
psi_list[[k]] <- NNiW[["psi"]]</pre>
S_list[[k]] <- NNiW[["S"]]</pre>
mmsNiWlogpdf(U_xi=xi_list, U_psi=psi_list, U_Sigma=S_list,
            U_xi0=list(hyperG0$b_xi), U_psi0=list(hyperG0$b_psi) ,
            U_B0=list(diag(c(hyperG0$D_xi, hyperG0$D_psi))) ,
            U_Sigma0=list(hyperG0$lambda), U_df0=list(hyperG0$nu))
hyperG0 <- list()</pre>
hyperG0$b_xi <- c(-1.6983129)
hyperG0$b_psi <- c(-0.0641866)
hyperG0$kappa <- 0.001
hyperG0$D_xi <- 16.951313
hyperG0$D_psi <- 1.255192
hyperG0$nu <- 27.67656
hyperG0$lambda <- matrix(c(2.3397761), ncol=1)
#'xi_list <- list()</pre>
psi_list <- list()</pre>
S_list <- list()</pre>
for(k in 1:1000){
NNiW <- rNNiW(hyperG0, diagVar=FALSE)
xi_list[[k]] <- NNiW[["xi"]]</pre>
psi_list[[k]] <- NNiW[["psi"]]</pre>
S_list[[k]] <- NNiW[["S"]]</pre>
}
mmsNiWlogpdf(U_xi=xi_list, U_psi=psi_list, U_Sigma=S_list,
            U_xi0=list(hyperG0$b_xi), U_psi0=list(hyperG0$b_psi) ,
            U_B0=list(diag(c(hyperG0$D_xi, hyperG0$D_psi))) ,
            U_Sigma0=list(hyperG0$lambda), U_df0=list(hyperG0$nu))
```

mmsNiWpdfC

C++ implementation of multivariate structured Normal inverse Wishart probability density function for multiple inputs

## **Description**

C++ implementation of multivariate structured Normal inverse Wishart probability density function for multiple inputs

## Usage

```
mmsNiWpdfC(xi, psi, Sigma, U_xi0, U_psi0, U_B0, U_Sigma0, U_df0, Log = TRUE)
```

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## **Arguments**

| xi       | data matrix of dimensions $p \times n$ where columns contain the observed mean vectors.  |
|----------|--|
| psi      | data matrix of dimensions $p \times n$ where columns contain the observed skew parameter vectors.  |
| Sigma    | list of length n of observed variance-covariance matrices, each of dimensions p $\mathbf{x}$ p.  |
| U_xi0    | mean vectors matrix of dimension $p \times K$ , $K$ being the number of distributions for which the density probability has to be evaluated. |
| U_psi0   | skew parameter vectors matrix of dimension p x K.  |
| U_B0     | list of length K of structured scale matrices, each of dimensions p x p.   |
| U_Sigma0 | list of length K of variance-covariance matrices, each of dimensions p x p.  |
| U_df0    | vector of length K of degree of freedom parameters.  |
| Log      | logical flag for returning the log of the probability density function. Defaults is TRUE.  |

# Value

matrix of densities of dimension K x n

## References

Hejblum BP, Alkhassim C, Gottardo R, Caron F and Thiebaut R (2019) Sequential Dirichlet Process Mixtures of Multivariate Skew t-distributions for Model-based Clustering of Flow Cytometry Data. The Annals of Applied Statistics, 13(1): 638-660. <doi: 10.1214/18-AOAS1209>. <arXiv: 1702.04407>. https://arxiv.org/abs/1702.04407 doi:10.1214/18AOAS1209

| mmvnpdfC | C++ implementation of multivariate Normal probability density function for multiple inputs |
|----------|--|
|          |  |

# Description

C++ implementation of multivariate Normal probability density function for multiple inputs

# Usage

```
mmvnpdfC(x, mean, varcovM, Log = TRUE)
```

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#### **Arguments**

x data matrix of dimension p x n, p being the dimension of the data and n the number of data points.

mean mean vectors matrix of dimension p x K, K being the number of distributions for which the density probability has to be evaluated.

varcovM list of length K of variance-covariance matrices, each of dimensions p x p.

Log logical flag for returning the log of the probability density function. Defaults is TRUE.

### Value

matrix of densities of dimension K x n.

## **Examples**

```
if(require(microbenchmark)){
library(microbenchmark)
microbenchmark(mvnpdf(x=matrix(1.96), mean=0, varcovM=diag(1), Log=FALSE),
               mvnpdfC(x=matrix(1.96), mean=0, varcovM=diag(1), Log=FALSE),
             mmvnpdfC(x=matrix(1.96), mean=matrix(0), varcovM=list(diag(1)), Log=FALSE),
               times=1000L)
microbenchmark(mvnpdf(x=matrix(rep(1.96,2), nrow=2, ncol=1), mean=c(-0.2, 0.3),
                      varcovM=matrix(c(2, 0.2, 0.2, 2), ncol=2), Log=FALSE),
              mvnpdfC(x=matrix(rep(1.96,2), nrow=2, ncol=1), mean=c(-0.2, 0.3),
                       varcovM=matrix(c(2, 0.2, 0.2, 2), ncol=2), Log=FALSE),
              mmvnpdfC(x=matrix(rep(1.96,2), nrow=2, ncol=1),
                        mean=matrix(c(-0.2, 0.3), nrow=2, ncol=1),
                        varcovM=list(matrix(c(2, 0.2, 0.2, 2), ncol=2)), Log=FALSE),
               times=1000L)
microbenchmark(mvnpdf(x=matrix(c(rep(1.96,2),rep(0,2)), nrow=2, ncol=2),
                      mean=list(c(0,0),c(-1,-1), c(1.5,1.5)),
                      varcovM=list(diag(2),10*diag(2), 20*diag(2)), Log=FALSE),
              mmvnpdfC(matrix(c(rep(1.96,2),rep(0,2)), nrow=2, ncol=2),
                        mean=matrix(c(0,0,-1,-1, 1.5,1.5), nrow=2, ncol=3),
                        varcovM=list(diag(2),10*diag(2), 20*diag(2)), Log=FALSE),
               times=1000L)
}else{
cat("package 'microbenchmark' not available\n")
```

mmvsnpdfC

C++ implementation of multivariate skew Normal probability density function for multiple inputs

### **Description**

C++ implementation of multivariate skew Normal probability density function for multiple inputs

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## Usage

```
mmvsnpdfC(x, xi, psi, sigma, Log = TRUE)
```

### **Arguments**

| x     | data matrix of dimension $p \times n$ , $p$ being the dimension of the data and $n$ the number of data points.                               |
|-------|--|
| xi    | mean vectors matrix of dimension $p \times K$ , $K$ being the number of distributions for which the density probability has to be evaluated. |
| psi   | skew parameter vectors matrix of dimension p x K.  |
| sigma | list of length K of variance-covariance matrices, each of dimensions p x p.  |
| Log   | logical flag for returning the log of the probability density function. Default is TRUE.   |

#### Value

matrix of densities of dimension K x n.

#### Author(s)

Boris Hejblum

```
mmvsnpdfC(x=matrix(rep(1.96,2), nrow=2, ncol=1),
                          xi=matrix(c(0, 0)), psi=matrix(c(1, 1),ncol=1), sigma=list(diag(2)), Log=FALSE
mmvsnpdfC(x=matrix(rep(1.96,2), nrow=2, ncol=1),
                          xi=matrix(c(0, 0)), psi=matrix(c(1, 1), ncol=1), sigma=list(diag(2))
if(require(microbenchmark)){
library(microbenchmark)
microbenchmark(mvsnpdf(x=matrix(rep(1.96,2), nrow=2, ncol=1), xi=c(0, 0), psi=c(1, 1), microbenchmark(mvsnpdf(x=matrix(rep(1.96,2), nrow=2, ncol=1), xi=c(0, 0), xi=c(0, 0),
                                                                  sigma=diag(2), Log=FALSE),
                                          mmvsnpdfC(x=matrix(rep(1.96,2), nrow=2, ncol=1), xi=matrix(c(0, 0)),
                                                                        psi=matrix(c(1, 1),ncol=1), sigma=list(diag(2)), Log=FALSE),
                                           times=1000L
microbenchmark(mvsnpdf(x=matrix(c(rep(1.96,2),rep(0,2)), nrow=2, ncol=2),
                                                               xi=list(c(0,0),c(-1,-1), c(1.5,1.5)),
                                                               psi=list(c(0.1,0.1),c(-0.1,-1), c(0.5,-1.5)),
                                                               sigma=list(diag(2),10*diag(2), 20*diag(2)), Log=FALSE),
                                          mmvsnpdfC(matrix(c(rep(1.96,2),rep(0,2)), nrow=2, ncol=2),
                                                                        xi=matrix(c(0,0,-1,-1, 1.5,1.5), nrow=2, ncol=3),
                                                                        psi=matrix(c(0.1,0.1,-0.1,-1, 0.5,-1.5), nrow=2, ncol=3),
                                                                        sigma=list(diag(2),10*diag(2), 20*diag(2)), Log=FALSE),
                                         times=1000L)
}else{
cat("package 'microbenchmark' not available\n")
```

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}

| mmvstpdfC | C++ implementation of multivariate Normal probability density func- |
|-----------|---|
|           | tion for multiple inputs  |

## **Description**

C++ implementation of multivariate Normal probability density function for multiple inputs

## Usage

```
mmvstpdfC(x, xi, psi, sigma, df, Log = TRUE)
```

## **Arguments**

| X     | data matrix of dimension $p \times n$ , $p$ being the dimension of the data and $n$ the number of data points.                               |
|-------|--|
| xi    | mean vectors matrix of dimension $p \times K$ , $K$ being the number of distributions for which the density probability has to be evaluated. |
| psi   | skew parameter vectors matrix of dimension p x K.  |
| sigma | list of length K of variance-covariance matrices, each of dimensions p x p.  |
| df    | vector of length K of degree of freedom parameters.  |
| Log   | logical flag for returning the log of the probability density function. Defaults is TRUE.  |

#### Value

matrix of densities of dimension K x n.

#### Author(s)

Boris Hejblum

```
mmvstpdfC(x = matrix(c(3.399890,-5.936962), ncol=1), xi=matrix(c(0.2528859,-2.4234067)),
psi=matrix(c(11.20536,-12.51052), ncol=1),
sigma=list(matrix(c(0.2134011, -0.0382573, -0.0382573, 0.2660086), ncol=2)),
df=c(7.784106)
)
mvstpdf(x = matrix(c(3.399890,-5.936962), ncol=1), xi=c(0.2528859,-2.4234067),
psi=c(11.20536,-12.51052),
sigma=matrix(c(0.2134011, -0.0382573, -0.0382573, 0.2660086), ncol=2),
df=c(7.784106)
)
```

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```
#skew-normal limit
mmvsnpdfC(x=matrix(rep(1.96,2), nrow=2, ncol=1),
         xi=matrix(c(0, 0)), psi=matrix(c(1, 1), ncol=1), sigma=list(diag(2))
mvstpdf(x=matrix(rep(1.96,2), nrow=2, ncol=1),
       xi=c(0, 0), psi=c(1, 1), sigma=diag(2),
       df=100000000
mmvstpdfC(x=matrix(rep(1.96,2), nrow=2, ncol=1),
         xi=matrix(c(0, 0)), psi=matrix(c(1, 1), ncol=1), sigma=list(diag(2)),
         df=100000000
         )
#non-skewed limit
mmvtpdfC(x=matrix(rep(1.96,2), nrow=2, ncol=1),
        mean=matrix(c(0, 0)), varcovM=list(diag(2)),
        df=10
        )
mmvstpdfC(x=matrix(rep(1.96,2), nrow=2, ncol=1),
         xi=matrix(c(0, 0)), psi=matrix(c(0, 0), ncol=1), sigma=list(diag(2)),
         )
if(require(microbenchmark)){
library(microbenchmark)
microbenchmark(mvstpdf(x=matrix(rep(1.96,2), nrow=2, ncol=1),
                       xi=c(0, 0), psi=c(1, 1),
                       sigma=diag(2), df=10),
               mmvstpdfC(x=matrix(rep(1.96,2), nrow=2, ncol=1),
                         xi=matrix(c(0, 0)), psi=matrix(c(1, 1), ncol=1),
                         sigma=list(diag(2)), df=10),
               times=1000L)
}else{
cat("package 'microbenchmark' not available\n")
```

mmvtpdfC

C++ implementation of multivariate Normal probability density function for multiple inputs

#### **Description**

C++ implementation of multivariate Normal probability density function for multiple inputs

```
mmvtpdfC(x, mean, varcovM, df, Log = TRUE)
```

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#### **Arguments**

x data matrix of dimension p x n, p being the dimension of the data and n the

number of data points.

mean vectors matrix of dimension p x K, K being the number of distributions for

which the density probability has to be evaluated.

varcovM list of length K of variance-covariance matrices, each of dimensions p x p.

df vector of length K of degree of freedom parameters.

Log logical flag for returning the log of the probability density function. Defaults is

TRUE.

#### Value

matrix of densities of dimension K x n.

#### Author(s)

Boris Hejblum

```
mvnpdf(x=matrix(1.96), mean=0, varcovM=diag(1), Log=FALSE)
mvtpdf(x=matrix(1.96), mean=0, varcovM=diag(1), df=10000000, Log=FALSE)
mmvtpdfC(x=matrix(1.96), mean=matrix(0), varcovM=list(diag(1)), df=10000000, Log=FALSE)
mvnpdf(x=matrix(1.96), mean=0, varcovM=diag(1))
mvtpdf(x=matrix(1.96), mean=0, varcovM=diag(1), df=10000000)
mmvtpdfC(x=matrix(1.96), mean=matrix(0), varcovM=list(diag(1)), df=10000000)
mvtpdf(x=matrix(1.96), mean=0, varcovM=diag(1), df=10)
mmvtpdfC(x=matrix(1.96), mean=matrix(0), varcovM=list(diag(1)), df=10)
if(require(microbenchmark)){
library(microbenchmark)
microbenchmark(mvtpdf(x=matrix(1.96), mean=0, varcovM=diag(1), df=1, Log=FALSE),
              mmvtpdfC(x=matrix(1.96), mean=matrix(0), varcovM=list(diag(1)),
                        df=c(1), Log=FALSE),
               times=10000L)
}else{
cat("package 'microbenchmark' not available\n")
```

mvnlikC75

| mvnlikC | C++ implementation of multivariate Normal probability density function for multiple inputs |
|---------|--|
|         |  |

## Description

C++ implementation of multivariate Normal probability density function for multiple inputs

## Usage

```
mvnlikC(x, c, clustval, mu, sigma, loglik = TRUE)
```

## Arguments

| X        | data matrix of dimension $p \times n$ , $p$ being the dimension of the data and $n$ the number of data points                  |
|----------|--|
| С        | integer vector of cluster allocations with values from 1 to K  |
| clustval | vector of unique values from c in the order corresponding to the storage of cluster parameters in $xi$ , $psi$ , and $varcovM$ |
| mu       | mean vectors matrix of dimension p x K, K being the number of clusters   |
| sigma    | list of length K of variance-covariance matrices, each of dimensions p x p.  |
| loglik   | logical flag or returning the log-likelihood instead of the likelihood. Default is TRUE.                                       |

#### Value

a list:

"indiv": vector of likelihood of length n; "clust": vector of likelihood of length K; "total":

total (log)-likelihood;

## Boris Hejblum

Author(s)

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| mν | n | p | d | f |
|----|---|---|---|---|
|    |   |   |   |   |

multivariate-Normal probability density function

## Description

multivariate-Normal probability density function

#### Usage

```
mvnpdf(x, mean, varcovM, Log = TRUE)
```

#### **Arguments**

x p x n data matrix with n the number of observations and p the number of dimen-

sions

mean vector or list of mean vectors (either a vector, a matrix or a list)

varcovM variance-covariance matrix or list of variance-covariance matrices (either a ma-

trix or a list)

Log logical flag for returning the log of the probability density function. Defaults is

TRUE.

#### Author(s)

Boris P. Hejblum

#### See Also

```
mvnpdf, mmvnpdfC
```

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| mvnpdfC | C++ implementation of multivariate normal probability density function for multiple inputs |
|---------|--|
|         |  |

#### **Description**

Based on the implementation from Nino Hardt and Dicko Ahmadou https://gallery.rcpp.org/articles/dmvnorm\_arma/ (accessed in August 2014)

#### Usage

```
mvnpdfC(x, mean, varcovM, Log = TRUE)
```

#### Arguments

x data matrix mean mean vector

varcovM variance covariance matrix

Log logical flag for returning the log of the probability density function. Default is

TRUE

#### Value

vector of densities

#### Author(s)

Boris P. Hejblum

78 mvsnlikC

| mvsnlikC | C++ implementation of multivariate skew normal likelihood function for multiple inputs |
|----------|--|
|          | jep.iep.iii  |

## Description

C++ implementation of multivariate skew normal likelihood function for multiple inputs

## Usage

```
mvsnlikC(x, c, clustval, xi, psi, sigma, loglik = TRUE)
```

## Arguments

| x        | data matrix of dimension $p \ x \ n, \ p$ being the dimension of the data and $n$ the number of data points          |
|----------|--|
| С        | integer vector of cluster allocations with values from 1 to K  |
| clustval | vector of unique values from c in the order corresponding to the storage of cluster parameters in xi, psi, and sigma |
| xi       | mean vectors matrix of dimension p x K, K being the number of clusters   |
| psi      | skew parameter vectors matrix of dimension p x K   |
| sigma    | list of length K of variance-covariance matrices, each of dimensions p x p.  |
| loglik   | logical flag or returning the log-likelihood instead of the likelihood. Default is TRUE.                             |

#### Value

a list:

"indiv": vector of likelihood of length n;
"clust": vector of likelihood of length K;
"total": total (log)-likelihood;

## Author(s)

Boris Hejblum

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| mvs     | nr    | hd | f |
|---------|-------|----|---|
| 111 7 3 | ı ı þ | Ju |   |

multivariate Skew-Normal probability density function

#### **Description**

multivariate Skew-Normal probability density function

#### Usage

```
mvsnpdf(x, xi, sigma, psi, Log = TRUE)
```

#### **Arguments**

| X     | $p \ x \ n$ data matrix with n the number of observations and p the number of dimensions       |
|-------|--|
| xi    | mean vector or list of mean vectors (either a vector, a matrix or a list)                      |
| sigma | variance-covariance matrix or list of variance-covariance matrices (either a matrix or a list) |
| psi   | skew parameter vector or list of skew parameter vectors (either a vector, a matrix or a list)  |
| Log   | logical flag for returning the log of the probability density function. Defaults is TRUE.      |

#### See Also

```
mvnpdf, mmvsnpdfC
```

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```
nu <- 1.5
W <- rgamma(n=N, shape=nu/2, rate=nu/2)</pre>
Yst=Ysn/sqrt(W)
library(reshape2)
library(ggplot2)
data2plot <- melt(cbind.data.frame(Ysn, Yst))</pre>
#pdf(file="ExSNST.pdf", height=5, width=4)
p <- (ggplot(data=data2plot)</pre>
     + geom_density(aes(x=value, fill=variable, alpha=variable), col="black")#, lwd=1.1)
     + theme_bw()
     + xlim(-15, 100)
     + theme(legend.position="bottom")
     + scale_fill_manual(values=alpha(c("#F8766D", "#00B0F6"),c(0.2,0.45)),
                          name =",
                          labels=c("Y~SN(0,1,10)
                                                       ", "Y~ST(0,1,10,1.5)")
     )
     + scale_alpha_manual(guide=FALSE, values=c(0.25, 0.45))
     + xlab("Y")
     + ylim(0,0.08)
     + ylab("Density")
     + guides(fill = guide_legend(override.aes = list(colour = NULL)))
     + theme(legend.key = element_rect(colour = "black"))
)
#dev.off()
```

mvstlikC

C++ implementation of multivariate skew t likelihood function for multiple inputs

#### Description

C++ implementation of multivariate skew t likelihood function for multiple inputs

#### Usage

```
mvstlikC(x, c, clustval, xi, psi, sigma, df, loglik = TRUE)
```

#### **Arguments**

x data matrix of dimension p x n, p being the dimension of the data and n the number of data points

c integer vector of cluster allocations with values from 1 to K

clustval vector of unique values from c in the order corresponding to the storage of cluster parameters in xi, psi, and sigma

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| xi     | mean vectors matrix of dimension p x K, K being the number of clusters                   |
|--------|--|
| psi    | skew parameter vectors matrix of dimension p x K   |
| sigma  | list of length K of variance-covariance matrices, each of dimensions p x p.              |
| df     | vector of length K of degree of freedom parameters.                                      |
| loglik | logical flag or returning the log-likelihood instead of the likelihood. Default is TRUE. |

## Value

a list:

"indiv": vector of likelihood of length n;
"clust": vector of likelihood of length K;
"total": total (log)-likelihood;

## Author(s)

Boris Hejblum

| mvstpdf | multivariate skew-t probability density function |  |
|---------|--|--|
|         |  |  |

## Description

multivariate skew-t probability density function

## Usage

```
mvstpdf(x, xi, sigma, psi, df, Log = TRUE)
```

## Arguments

| Х     | p x n data matrix with n the number of observations and p the number of dimensions             |
|-------|--|
| xi    | mean vector or list of mean vectors (either a vector, a matrix or a list)                      |
| sigma | variance-covariance matrix or list of variance-covariance matrices (either a matrix or a list) |
| psi   | skew parameter vector or list of skew parameter vectors (either a vector, a matrix or a list)  |
| df    | a numeric vector or a list of the degrees of freedom (either a vector or a list)               |
| Log   | logical flag for returning the log of the probability density function. Defaults is TRUE.      |

## See Also

```
mvtpdf, mvsnpdf, mmvstpdfC, mvstlikC
```

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#### **Examples**

mvtpdf

multivariate Student's t-distribution probability density function

#### **Description**

multivariate Student's t-distribution probability density function

## Usage

```
mvtpdf(x, mean, varcovM, df, Log = TRUE)
```

#### **Arguments**

| X       | $p \; x \; n$ data matrix with $n$ the number of observations and $p$ the number of dimensions |
|---------|--|
| mean    | mean vector or list of mean vectors (either a vector, a matrix or a list)                      |
| varcovM | variance-covariance matrix or list of variance-covariance matrices (either a matrix or a list) |
| df      | a numeric vector or a list of the degrees of freedom (either a vector or a list)               |
| Log     | logical flag for returning the log of the probability density function. Defaults is            |

```
mvtpdf(x=matrix(1.96), mean=0, varcovM=diag(1), df=10000000)
mvnpdf(x=matrix(1.96), mean=0, varcovM=diag(1))
mvtpdf(x=matrix(1.96), mean=0, varcovM=diag(1), df=10)
```

NuMatParC 83

NuMatParC

C++ implementation of similarity matrix computation using precomputed distances

## Description

C++ implementation of similarity matrix computation using pre-computed distances

## Usage

```
NuMatParC(c, d)
```

## Arguments

c an MCMC partitions of length n.

d a symmetric n x n matrix containing distances between each group distributions.

#### Author(s)

Boris Hejblum, Chariff Alkhassim

## **Examples**

```
c <- c(1,1,2,3,2,3)
d <- matrix(runif(length(c)^2),length(c))
NuMatParC(c,d)</pre>
```

plot\_ConvDPM

Convergence diagnostic plots

## Description

Convergence diagnostic plots

plot\_DPM

#### Usage

```
plot_ConvDPM(
   MCMCsample,
   from = 1,
   to = length(MCMCsample$logposterior_list),
   shift = 0,
   thin = 1,
   ...
)
```

#### **Arguments**

MCMCsample a DPMMclust or summaryDPMMclust object.

from the MCMC iteration from which the plot should start. Default is 1.

to the MCMC iteration up until which the plot should stop. Default is 1.

shift a number of initial iterations not to be displayed. Default is 0.

thin integer giving the spacing at which MCMC iterations are kept. Default is 1, i.e. no thining.

... further arguments passed to or from other methods

plot\_DPM

Plot of a Dirichlet process mixture of gaussian distribution partition

#### **Description**

Plot of a Dirichlet process mixture of gaussian distribution partition

```
plot_DPM(
    z,
    U_mu = NULL,
    U_Sigma = NULL,
    m,
    c,
    i,
    alpha = "?",
    U_SS = NULL,
    dims2plot = 1:nrow(z),
    ellipses = ifelse(length(dims2plot) < 3, TRUE, FALSE),
    gg.add = list(theme())
)</pre>
```

plot\_DPMsn 85

## Arguments

| Z         | data matrix d x n with d dimensions in rows and n observations in columns.  |
|-----------|---|
| U_mu      | either a list or a matrix containing the current estimates of mean vectors of length d for each cluster. Default is NULL in which case U_SS has to be provided.       |
| U_Sigma   | either a list or an array containing the $d \times d$ current estimates for covariance matrix of each cluster. Default is NULL in which case U_SS has to be provided. |
| m         | vector of length $\boldsymbol{n}$ containing the number of observations currently assigned to each clusters.  |
| С         | allocation vector of length $\boldsymbol{n}$ indicating which observation belongs to which clusters.  |
| i         | current MCMC iteration number.  |
| alpha     | current value of the DP concentration parameter.  |
| U_SS      | a list containing "mu" and "S". Default is NULL in which case $U_mu$ and $U_Sigma$ have to be provided.   |
| dims2plot | index vector, subset of $1:d$ indicating which dimensions should be drawn. Default is all of them.  |
| ellipses  | a logical flag indicating whether ellipses should be drawn around clusters. Default is TRUE if only 2 dimensions are plotted, FALSE otherwise.                        |
| gg.add    | a list of instructions to add to the ggplot2 instruction (see gg-add). Default is list(theme()), which adds nothing to the plot.                                      |

## Author(s)

Boris Hejblum

| plot_DPMsn | Plot of a Dirichlet process mixture of skew normal distribution partition |
|------------|---|
|            |   |

## Description

Plot of a Dirichlet process mixture of skew normal distribution partition

```
plot_DPMsn(
   z,
   c,
   i = "",
   alpha = "?",
   U_SS,
   dims2plot = 1:nrow(z),
   ellipses = ifelse(length(dims2plot) < 3, TRUE, FALSE),
   gg.add = list(theme()),
   nbsim_dens = 1000
)</pre>
```

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## **Arguments**

| z          | data matrix d x n with d dimensions in rows and n observations in columns.   |
|------------|--|
| С          | allocation vector of length n indicating which observation belongs to which clusters.  |
| i          | current MCMC iteration number.   |
| alpha      | current value of the DP concentration parameter.   |
| U_SS       | a list containing "xi", "psi", "S", and "df".  |
| dims2plot  | index vector, subset of 1:d indicating which dimensions should be drawn. Default is all of them.   |
| ellipses   | a logical flag indicating whether ellipses should be drawn around clusters. Default is TRUE if only 2 dimensions are plotted, FALSE otherwise. |
| gg.add     | A list of instructions to add to the ggplot2 instruction (see gg-add). Default is list(theme()), which adds nothing to the plot.               |
| nbsim_dens | number of simulated points used for computing clusters density contours in 2D plots. Default is 1000 points.                                   |

## Author(s)

Boris Hejblum

plot\_DPMst

Plot of a Dirichlet process mixture of skew t-distribution partition

## Description

Plot of a Dirichlet process mixture of skew t-distribution partition

```
plot_DPMst(
    z,
    c,
    i = "",
    alpha = "?",
    U_SS,
    dims2plot = 1:nrow(z),
    ellipses = ifelse(length(dims2plot) < 3, TRUE, FALSE),
    gg.add = list(theme()),
    nbsim_dens = 1000,
    nice = FALSE
)</pre>
```

## Arguments

| Z          | data matrix d x n with d dimensions in rows and n observations in columns.   |
|------------|--|
| С          | allocation vector of length $\boldsymbol{n}$ indicating which observation belongs to which clusters.   |
| i          | current MCMC iteration number.   |
| alpha      | current value of the DP concentration parameter.   |
| U_SS       | a list containing "xi", "psi", "S", and "df".  |
| dims2plot  | index vector, subset of 1:d indicating which dimensions should be drawn. Default is all of them.   |
| ellipses   | a logical flag indicating whether ellipses should be drawn around clusters. Default is TRUE if only 2 dimensions are plotted, FALSE otherwise. |
| gg.add     | A list of instructions to add to the ggplot2 instruction (see gg-add). Default is list(theme()), which adds nothing to the plot.               |
| nbsim_dens | number of simulated points used for computing clusters density contours in 2D plots. Default is 1000 points.                                   |
| nice       | logical flag changing the plot looks. Default is FALSE.  |
|            |  |

## Author(s)

Boris Hejblum

## Description

Post-processing Dirichlet Process Mixture Models results to get a mixture distribution of the posterior locations

```
postProcess.DPMMclust(
    x,
    burnin = 0,
    thin = 1,
    gs = NULL,
    lossFn = "F-measure",
    K = 10,
    ...
)
```

#### **Arguments**

x a DPMMclust object.

burnin integer giving the number of MCMC iterations to burn (defaults is half)

thin integer giving the spacing at which MCMC iterations are kept. Default is 1, i.e.

no thining.

gs optional vector of length n containing the gold standard partition of the n obser-

vations to compare to the point estimate.

lossFn character string specifying the loss function to be used. Either "F-measure" or

"Binder" (see Details). Default is "F-measure".

K integer giving the number of mixture components. Default is 10.

... further arguments passed to or from other methods

#### **Details**

The cost of a point estimate partition is calculated using either a pairwise coincidence loss function (Binder), or 1-Fmeasure (F-measure).

#### Value

a list:

burnin: an integer passing along the burnin argument

thin: an integer passing along the thin argument

lossFn: a character string passing along the lossFn argument

point\_estim:

loss:

index\_estim:

## Author(s)

Boris Hejblum

#### See Also

similarityMat summary.DPMMclust

```
print.summaryDPMMclust
```

Methods for a summary of a DPMMclust object

#### **Description**

Methods for a summary of a DPMMclust object

## Usage

```
## S3 method for class 'summaryDPMMclust'
print(x, ...)
## S3 method for class 'summaryDPMMclust'
plot(
    x,
    hm = FALSE,
    nbsim_densities = 5000,
    hm_subsample = NULL,
    hm_order_by_clust = TRUE,
    gg.add = list(theme_bw()),
    ...
)
```

#### **Arguments**

x a summaryDPMMclust object.

... further arguments passed to or from other methods

hm logical flag to plot the heatmap of the similarity matrix. Default is FALSE.

nbsim\_densities

the number of simulated observations to be used to plot the density lines of the

clusters in the point estimate partition plot

hm\_subsample a integer designating the number of observations to use when plotting the heatmap.

Used only if hm is TRUE. #'Default is NULL in which no subsampling is done and

all observations are plotted.

hm\_order\_by\_clust

logical flag indicating whether observations should be ordered according to the

point estimate first. Used only if hm is TRUE. Default is TRUE.

gg.add a list of instructions to add to the ggplot2 instruction (see gg-add). Default is

list(theme()), which adds nothing to the plot.

#### Author(s)

Boris Hejblum

90 priormix

priormix

Construction of an Empirical based prior

#### **Description**

Construction of an Empirical based prior

#### Usage

```
priormix(sDPMclust, nu0add = 5)
```

## **Arguments**

sDPMclust an object of class summary.DPMMclust

nu0add an additional value integer added to hyperprior parameter nu (increase to avoid

non positive definite matrix sampling)

#### See Also

```
summary.DPMMclust
```

```
rm(list=ls())
#Number of data
n <- 2000
set.seed(123)
#set.seed(4321)
d <- 2
ncl <- 4
# Sample data
sdev <- array(dim=c(d,d,ncl))</pre>
xi <- matrix(nrow=d, ncol=ncl, c(-1.5, 1.5, 1.5, 1.5, 2, -2.5, -2.5, -3))
#xi <- matrix(nrow=d, ncol=ncl, c(-0.5, 0, 0.5, 0, 0.5, -1, -1, 1))</pre>
psi <- matrix(nrow=d, ncol=4, c(0.4, -0.6, 0.8, 0, 0.3, -0.7, -0.3, -0.8))
nu <- c(100, 15, 8, 5)
p <- c(0.15, 0.05, 0.5, 0.3) # frequence des clusters
sdev[, ,1] \leftarrow matrix(nrow=d, ncol=d, c(0.3, 0, 0, 0.3))
sdev[, ,2] <- matrix(nrow=d, ncol=d, c(0.1, 0, 0, 0.3))</pre>
sdev[, ,3] <- matrix(nrow=d, ncol=d, c(0.3, 0.15, 0.15, 0.3))</pre>
sdev[, ,4] <- .3*diag(2)
```

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```
c \leftarrow rep(0,n)
w \leftarrow rep(1,n)
z <- matrix(0, nrow=d, ncol=n)</pre>
for(k in 1:n){
c[k] = which(rmultinom(n=1, size=1, prob=p)!=0)
 w[k] \leftarrow rgamma(1, shape=nu[c[k]]/2, rate=nu[c[k]]/2)
 z[,k] \leftarrow xi[, c[k]] + psi[, c[k]]*rtruncnorm(n=1, a=0, b=Inf, mean=0, sd=1/sqrt(w[k])) +
            (sdev[, , c[k]]/sqrt(w[k]))%*\\ %matrix(rnorm(d, mean = 0, sd = 1), nrow=d, ncol=1)
 \#cat(k, "/", n, " observations simulated\n", sep="")
# Set parameters of G0
hyperG0 <- list()</pre>
hyperG0[["b_xi"]] <- rowMeans(z)</pre>
hyperG0[["b_psi"]] <- rep(0,d)
hyperG0[["kappa"]] <- 0.001
hyperG0[["D_xi"]] <- 100
hyperG0[["D_psi"]] <- 100
hyperG0[["nu"]] \leftarrow d+1
hyperG0[["lambda"]] <- diag(apply(z,MARGIN=1, FUN=var))/3
 # hyperprior on the Scale parameter of DPM
 a <- 0.0001
 b <- 0.0001
 nbclust_init <- 30</pre>
if(interactive()){
 MCMCsample_st <- DPMGibbsSkewT(z, hyperG0, a, b, N=2000, doPlot=FALSE,</pre>
                                   nbclust_init, diagVar=FALSE)
 s <- summary(MCMCsample_st, burnin = 1500, thin=5, posterior_approx=TRUE)</pre>
 pmix <- priormix(s)</pre>
```

rCRP

Generating cluster data from the Chinese Restaurant Process

#### **Description**

Generating cluster data from the Chinese Restaurant Process

## Usage

```
rCRP(n = 1000, alpha = 2, hyperG0, verbose = TRUE)
```

#### **Arguments**

```
n number of observations alpha concentration parameter
```

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hyperG0 base distribution hyperparameter

verbose logical flag indicating whether info is written in the console.

```
rm(list=ls())
d=2
hyperG0 <- list()</pre>
hyperG0[["NNiW"]] <- list()</pre>
hyperG0[["NNiW"]][["b_xi"]] <- rep(0,d)
hyperG0[["NNiW"]][["b_psi"]] <- rep(0,d)
hyperG0[["NNiW"]][["D_xi"]] <- 100
hyperG0[["NNiW"]][["D_psi"]] <- 8
hyperG0[["NNiW"]][["nu"]] <- d+1
hyperG0[["NNiW"]][["lambda"]] \leftarrow diag(c(1,1))
hyperG0[["scale"]] <- list()</pre>
set.seed(4321)
N <- 200
alph <- runif(n=1,0.2,2)
GvHD_sims <- rCRP(n=2*N, alpha=alph, hyperG0=hyperG0)</pre>
library(ggplot2)
q <- (ggplot(data=cbind.data.frame("D1"=GvHD_sims$data[1,],</pre>
                                    "D2"=GvHD_sims$data[2,],
                                    "Cluster"=GvHD_sims$cluster),
             aes(x=D1, y=D2))
      + geom_point(aes(colour=Cluster), alpha=0.6)
      + theme_bw()
#q + stat_density2d(alpha=0.15, geom="polygon")
if(interactive()){
MCMCy1 \leftarrow DPMGibbsSkewT(z=GvHD_sims$data[,1:N],
                         hyperG0$NNiW, a=0.0001, b=0.0001, N=5000,
                         doPlot=TRUE, nbclust_init=64, plotevery=500,
                         gg.add=list(theme_bw()), diagVar=FALSE)
 s1 <- summary(MCMCy1, burnin=4000, thin=5,</pre>
               posterior_approx=TRUE)
F1 <- FmeasureC(ref=GvHD_sims$cluster[1:N], pred=s1$point_estim$c_est)
 # s <- summary(MCMCy1, burnin=4000, thin=5,
                  posterior_approx=TRUE, K=1)
 # s2 <- summary(MCMCy1, burnin=4000, thin=5,</pre>
                  posterior_approx=TRUE, K=2)
 # MCMCy2_seqPost<- DPMGibbsSkewT(z=GvHD_sims$data[,(N+1):(2*N)],</pre>
 #
                                      hyperG0=s1$param_post$parameters,
 #
                                      a=s1$param_post$alpha_param$shape,
 #
                                      b=s1$param_post$alpha_param$rate,
```

sample\_alpha 93

```
N=5000, doPlot=TRUE, nbclust_init=64, plotevery=500,
                                                                                                     gg.add=list(theme_bw()), diagVar=FALSE)
MCMCy2_seqPost <- DPMGibbsSkewT_SeqPrior(z=GvHD_sims$data[,(N+1):(2*N)],</pre>
                                                                                                     prior=s1$param_post, hyperG0=hyperG0$NNiW, , N=1000,
                                                                                                                        doPlot=TRUE, nbclust_init=10, plotevery=100,
                                                                                                                        gg.add=list(theme_bw()), diagVar=FALSE)
 s2_seqPost <- summary(MCMCy2_seqPost, burnin=600, thin=2)</pre>
F2\_seqPost \leftarrow FmeasureC(ref=GvHD\_sims\\cluster[(N+1):(2*N)], pred=s2\_seqPost\\point\_estim\\sc\_est)
MCMCy2 <- DPMGibbsSkewT(z=GvHD_sims$data[,(N+1):(2*N)],</pre>
                                                                     hyperG0$NNiW, a=0.0001, b=0.0001, N=5000,
                                                                     doPlot=TRUE, nbclust_init=64, plotevery=500,
                                                                      gg.add=list(theme_bw()), diagVar=FALSE)
 s2 <- summary(MCMCy2, burnin=4000, thin=5)</pre>
 F2 <- FmeasureC(ref=GvHD_sims$cluster[(N+1):(2*N)], pred=s2$point_estim$c_est)
MCMCtot <- DPMGibbsSkewT(z=GvHD_sims$data,</pre>
                                                                        hyperG0$NNiW, a=0.0001, b=0.0001, N=5000,
                                                                        doPlot=TRUE, nbclust_init=10, plotevery=500,
                                                                        gg.add=list(theme_bw()), diagVar=FALSE)
stot <- summary(MCMCtot, burnin=4000, thin=5)</pre>
\label{eq:f2tot} F2tot <- FmeasureC(ref=GvHD\_sims$cluster[(N+1):(2*N)], pred=stot$point\_estim$c_est[(N+1):(2*N)])$ and the sum of the stot of the st
c(F1, F2, F2_seqPost, F2tot)
```

sample\_alpha

Sampler for the concentration parameter of a Dirichlet process

#### **Description**

Sampler updating the concentration parameter of a Dirichlet process given the number of observations and a Gamma(a, b) prior, following the augmentation strategy of West, and of Escobar and West.

#### Usage

```
sample_alpha(alpha_old, n, K, a = 1e-04, b = 1e-04)
```

## Arguments

| alpha_old | the current value of alpha  |
|-----------|---|
| n         | the number of data points   |
| K         | current number of cluster   |
| a         | shape hyperparameter of the Gamma prior on the concentration parameter of the Dirichlet Process. Default is 0, 0001 |

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b

scale hyperparameter of the Gamma prior on the concentration parameter of the Dirichlet Process. Default is 0.0001. If 0 then the concentration is fixed and this function returns a.

#### **Details**

A Gamma prior is used.

#### References

M West, Hyperparameter estimation in Dirichlet process mixture models, Technical Report, Duke University, 1992.

MD Escobar, M West, Bayesian Density Estimation and Inference Using Mixtures *Journal of the American Statistical Association*, 90(430):577-588, 1995.

```
#Test with a fixed K
alpha_init <- 1000
N <- 10000
#n=500
n=10000
K <- 80
a <- 0.0001
b <- a
alphas <- numeric(N)</pre>
alphas[1] <- alpha_init
for (i in 2:N){
 alphas[i] <- sample_alpha(alpha_old = alphas[i-1], n=n, K=K, a=a, b=b)</pre>
postalphas <- alphas[floor(N/2):N]</pre>
alphaMMSE <- mean(postalphas)</pre>
alphaMAP <- density(postalphas)$x[which.max(density(postalphas)$y)]</pre>
expK <- sum(alphaMMSE/(alphaMMSE+0:(n-1)))</pre>
round(expK)
 prioralpha <- data.frame("alpha"=rgamma(n=5000, a,1/b),</pre>
                          "distribution" = factor(rep("prior", 5000),
                          levels=c("prior", "posterior")))
 library(ggplot2)
 p <- (ggplot(prioralpha, aes(x=alpha))</pre>
       + geom_histogram(aes(y=..density..),
                         colour="black", fill="white")
       + geom_density(alpha=.2, fill="red")
       + ggtitle(paste("Prior distribution on alpha: Gamma(", a,
                  ",", b, ")\n", sep=""))
```

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similarityMat

Computes the co-clustering (or similarity) matrix

## Description

Computes the co-clustering (or similarity) matrix

#### Usage

```
similarityMat(c, step = 1)
```

#### Arguments

c a list of vector of length n. c[[j]][i] is the cluster allocation of observation i=1...n at iteration j=1...N.

step provide co-clustering every step iterations. Default is 1.

#### Value

A matrix of size  $n \times n$  whose term [i,j] is the proportion of MCMC iterations where observation i and observations j are allocated to the same cluster.

#### Author(s)

Boris Hejblum

similarityMatC

C++ implementation

## Description

C++ implementation

#### Usage

```
similarityMatC(cc)
```

#### **Arguments**

СС

a matrix whose columns each represents a (MCMC) partition

## **Examples**

```
c <- list(c(1,1,2,3,2,3), c(1,1,1,2,3,3),c(2,2,1,1,1,1))
similarityMatC(sapply(c, "["))

c2 <- list()
for(i in 1:10){
      c2 <- c(c2, list(rmultinom(n=1, size=200, prob=rexp(n=200))))
}
similarityMatC(sapply(c2, "["))</pre>
```

 $similarityMat_nocostC$  C++implementation

## Description

C++ implementation

## Usage

```
similarityMat_nocostC(cc)
```

#### **Arguments**

 $\mathsf{CC}$ 

a matrix whose columns each represents a ()MCMC) partition

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#### **Examples**

```
c <- list(c(1,1,2,3,2,3), c(1,1,1,2,3,3),c(2,2,1,1,1,1))
similarityMat_nocostC(sapply(c, "["))

c2 <- list()
for(i in 1:10){
      c2 <- c(c2, list(rmultinom(n=1, size=1000, prob=rexp(n=1000))))
}

c3 <- sapply(c2, "[")

if(require(microbenchmark)){
library(microbenchmark)
microbenchmark(similarityMat(c3), similarityMat_nocostC(c3), times=2L)
}else{
cat("package 'microbenchmark' not available\n")
}</pre>
```

summary.DPMMclust

Summarizing Dirichlet Process Mixture Models

#### **Description**

Summary methods for DPMMclust objects.

#### Usage

```
## S3 method for class 'DPMMclust'
summary(
  object,
  burnin = 0,
  thin = 1,
  gs = NULL,
  lossFn = "Binder",
  posterior_approx = FALSE,
   ...
)
```

#### **Arguments**

object a DPMMclust object.

burnin integer giving the number of MCMC iterations to burn (defaults is half)

thin integer giving the spacing at which MCMC iterations are kept. Default is 1, i.e. no thining.

gs optional vector of length n containing the gold standard partition of the n obser-

vations to compare to the point estimate

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lossFn character string specifying the loss function to be used. Either "F-measure" or "Binder" (see Details). Default is "Binder".

posterior\_approx

logical flag whether a parametric approximation of the posterior should be computed. Default is FALSE

... further arguments passed to or from other methods

#### **Details**

The cost of a point estimate partition is calculated using either a pairwise coincidence loss function (Binder), or 1-Fmeasure (F-measure).

The number of retained sampled partitions is m = (N - burnin)/thin

#### Value

a list containing the following elements:

nb\_mcmcit: an integer giving the value of m, the number of retained sampled partitions, i.e. (N - burnin)/thin

burnin: an integer passing along the burnin argument

thin: an integer passing along the thin argument

lossFn: a character string passing along the lossFn argument

clust\_distrib: a character string passing along the clust\_distrib argument

point\_estim: a list containing:

c\_est: a vector of length ncontaining the point estimated clustering for each observations

cost: a vector of length m containing the cost of each sampled partition

Fmeas: if lossFn is 'F-measure', the m x m matrix of total F-measures for each pair of sampled partitions

opt\_ind: the index of the point estimate partition among the m sampled

loss: the loss for the point estimate. NA if lossFn is not 'Binder'

param\_posterior: a list containing the parametric approximation of the posterior, suitable to be plugged in as prior for a new MCMC algorithm run

mcmc\_partitions: a list containing the m sampled partitions

alpha: a vector of length m with the values of the alpha DP parameter

index\_estim: the index of the point estimate partition among the m sampled

hyperGO: a list passing along the prior, i.e. the hyperGO argument

logposterior\_list: a list of length m containing the logposterior and its decomposition, for each sampled partition

U\_SS\_list: a list of length m containing the containing the lists of sufficient statistics for all the mixture components, for each sampled partition

data: a d x n matrix containing the clustered data

#### Author(s)

Boris Hejblum

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## See Also

 ${\tt similarityMat\ similarityMatC}$ 

vclust2mcoclustC

C++ implementation

## Description

C++ implementation

## Usage

vclust2mcoclustC(c)

## Arguments

С

is an MCMC partition

## Author(s)

Chariff Alkhassim

```
cc <- c(1,1,2,3,2,3)
vclust2mcoclustC(cc)</pre>
```

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