# Package 'fabMix'

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Type Package

**Title** Overfitting Bayesian Mixtures of Factor Analyzers with Parsimonious Covariance and Unknown Number of Components

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# **Description**

Model-based clustering of multivariate continuous data using Bayesian mixtures of factor analyzers (Papastamoulis (2018) <DOI:10.1016/j.csda.2018.03.007>). The number of clusters is estimated using overfitting mixture models (Rousseau and Mengersen (2011) <DOI:10.1111/j.1467-9868.2011.00781.x>): suitable prior assumptions ensure that asymptotically the extra components will have zero posterior weight, therefore, the inference is based on the "alive" components. A Gibbs sampler is implemented in order to (approximately) sample from the posterior distribution of the overfitting mixture. A prior parallel tempering scheme is also available, which allows to run multiple parallel chains with different prior distributions on the mixture weights. These chains run in parallel and can swap states using a Metropolis-Hastings move. Eight different parameterizations give rise to parsimonious representations of the covariance per cluster (following Mc Nicholas and Murphy (2008) <DOI:10.1007/s11222-008-9056-0>). The model parameterization and number of factors is selected according to the Bayesian Information Criterion. Identifiability issues related to label switching are dealt by post-processing the simulated output with the Equivalence Classes Representatives algorithm (Papastamoulis and Iliopoulos (2010) <a href="https://www.jstor.org/stable/25703571">https://www.jstor.org/stable/25703571</a>, Papastamoulis (2016) <DOI:10.18637/jss.v069.c01>).

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URL https://github.com/mqbssppe/overfittingFABMix

**Imports** Rcpp (>= 0.12.17), MASS, doParallel, foreach, label.switching, mvtnorm, doRNG, RColorBrewer, corrplot, mclust, coda, ggplot2

LinkingTo Rcpp, RcppArmadillo

NeedsCompilation yes

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# $\mathsf{R}$ topics documented:

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fabMix-package

Overfitting Bayesian Mixtures of Factor Analyzers with Parsimonious Covariance and Unknown Number of Components

### Description

Model-based clustering of multivariate continuous data using Bayesian mixtures of factor analyzers (Papastamoulis (2018) <DOI:10.1016/j.csda.2018.03.007>). The number of clusters is estimated using overfitting mixture models (Rousseau and Mengersen (2011) <DOI:10.1111/j.1467-9868.2011.00781.x>): suitable prior assumptions ensure that asymptotically the extra components will have zero posterior weight, therefore, the inference is based on the "alive" components. A Gibbs sampler is implemented in order to (approximately) sample from the posterior distribution of the overfitting mixture. A prior parallel tempering scheme is also available, which allows to run multiple parallel chains with different prior distributions on the mixture weights. These chains run in parallel and can swap states using a Metropolis-Hastings move. Eight different parameterizations give rise to parsimonious representations of the covariance per cluster (following Mc Nicholas and Murphy (2008) <DOI:10.1007/s11222-008-9056-0>). The model parameterization and number of factors is selected according to the Bayesian Information Criterion. Identifiability issues related to label switching are dealt by post-processing the simulated output with the Equivalence Classes Representatives algorithm (Papastamoulis and Iliopoulos (2010) <a href="https://www.jstor.org/stable/25703571">https://www.jstor.org/stable/25703571</a>, Papastamoulis (2016) <DOI:10.18637/jss.v069.c01>).

The main fuction of the package is fabMix.

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### Author(s)

Panagiotis Papastamoulis

Maintainer: Panagiotis Papastamoulis <papapast@yahoo.gr>

### References

Fokoue, E. and Titterington, D.M. (2003). Mixtures of Factor Analysers: Bayesian Estimation and Inference by Stochastic Simulation. Machine Learning, 50(1): 73-94.

McNicholas, P.D. and Murphy, T.B. Statistics and Computing (2008) 18: 285. https://doi.org/10.1007/s11222-008-9056-0.

Papastamoulis P. and Iliopoulos G. (2010). An artificial allocations based solution to the label switching problem in Bayesian analysis of mixtures of distributions. Journal of Computational and Graphical Statistics, 19: 313-331.

Rousseau, J. and Mengersen, K. (2011). Asymptotic behaviour of the posterior distribution in overfitted mixture models. Journal of the Royal Statistical Society, Series B (methodological), 73(5): 689-710.

van Havre, Z., White, N., Rousseau, J. and Mengersen, K. (2015). Overfitting Bayesian Mixture Models with an Unknown Number of Components. PLOS ONE, 10(7): 1-27.

Papastamoulis, P. (2016). label.switching: An R Package for Dealing with the Label Switching Problem in MCMC Outputs. Journal of Statistical Software, 69(1), 1-24.

Papastamoulis, P. (2018). Overfitting Bayesian mixtures of factor analyzers with an unknown number of components. Computational Statistics and Data Analysis, 124: 220-234. DOI: 10.1016/j.csda.2018.03.007.

### See Also

```
fabMix, plot.fabMix.object
```

### **Examples**

```
# TOY EXAMPLE (very small numbers... only for CRAN check purposes)
# (a) using 2 cores in parallel, each one running 2 heated chains.
library('fabMix')
n = 8
                 # sample size
                 # number of variables
p = 5
q = 2
                 # number of factors
K = 2
        # true number of clusters
sINV_diag = 1/((1:p)) # diagonal of inverse variance of errors
set.seed(100)
syntheticDataset <- simData(sameLambda=TRUE,K.true = K, n = n, q = q, p = p,
sINV_values = sINV_diag)
colnames(syntheticDataset$data) <- paste0("x_",1:p)</pre>
# Run `fabMix` for a _small_ number of iterations for the
```

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```
# `UUU` (maximal model) and `CCC` (minimal model) parameterizations,
# using the default prior parallel heating parameters `dirPriorAlphas`.
# NOTE: `dirPriorAlphas` may require some tuning in general.
qRange <- 2 # values for the number of factors (only the true number
                                                 is considered here)
Kmax <- 4 # number of components for the overfitted mixture model
nChains <- 2 # number of parallel heated chains
set.seed(1)
fm <- fabMix( model = c("UUU", "CCC"), nChains = nChains,</pre>
rawData = syntheticDataset$data, outDir = "toyExample",
       Kmax = Kmax, mCycles = 4, burnCycles = 1, q = qRange,
       g = 0.5, h = 0.5, alpha_sigma = 0.5, beta_sigma = 0.5,
       warm_up_overfitting = 2, warm_up = 5)
# WARNING: the following parameters:
# Kmax, nChains, mCycles, burnCycles, warm_up_overfitting, warm_up
  should take (much) _larger_ values. E.g. a typical implementation consists of:
        Kmax = 20, nChains >= 3, mCycles = 1100, burnCycles = 100,
        warm_up_overfitting = 500, warm_up = 5000.
# Now print a run summary and produce some plots.
print(fm)
plot(fm, what = "BIC")
# (b) using 12 cores___
#_____4 models with 3 heated chains running in parallel_____
#_____considering all 8 model parameterizations_____
## Not run:
library('fabMix')
set.seed(99)
n = 100
                    # sample size
p = 30
                   # number of variables
                   # number of factors
q = 2
K = 5 # number of clusters
sINV_diag = rep(1/100,p) # diagonal of inverse variance of errors
syntheticDataset <- simData(sameLambda=FALSE, K.true = K, n = n, q = q, p = p,
sINV_values = sINV_diag)
colnames(syntheticDataset$data) <- paste0("x_",1:p)
qRange <- 1:3 # range of values for the number of factors
Kmax <- 20 # number of components for the overfitted mixture model
nChains <- 3 # number of parallel heated chains
# the next command takes \sim 1 hour in a Linux workstation with 12 threads.
fm <- fabMix( parallelModels = 4,</pre>
nChains = nChains,
model = c("UUU","CUU","UCU","CCU","UCC","UUC","CUC","CCC"),
rawData = syntheticDataset$data, outDir = "toyExample_b",
       Kmax = Kmax, mCycles = 600, burnCycles = 100, q = qRange,
```

complete.log.likelihood

Complete log-likelihood function for xCx models.

# **Description**

Complete log-likelihood function for models with same error variance per component (xCx).

# Usage

```
complete.log.likelihood(x_data, w, mu, Lambda, SigmaINV, z)
```

# **Arguments**

x\_data  $n \times p$  matrix containing the data

w a vector of length K containing the mixture weights

mu  $K \times p$  matrix containing the marginal means per component

Lambda  $K \times p \times q$  array of factor loadings per component

SigmaINV  $p \times p$  precision matrix (inverse covariance)

z A vector of length n containing the allocations of the n datapoints to the K

mixture components

### Value

complete log-likelihood value

# Author(s)

```
library('fabMix')
data(waveDataset1500)
x_data <- waveDataset1500[ 1:20, -1] # data</pre>
z <- waveDataset1500[ 1:20, 1] # class</pre>
p \leftarrow dim(x_data)[2]
q <- 2
K <- length(table(z)) # 3 classes</pre>
# give some arbitrary values to the parameters:
set.seed(1)
w \leftarrow rep(1/K, K)
mu \leftarrow array(runif(K * p), dim = c(K,p))
Lambda <- array( runif(K*p*q), dim = c(K,p,q))
SigmaINV <- array(1, dim = c(p,p))
# compute the complete.log.likelihood
complete.log.likelihood(x_data = x_data, w = w, mu = mu,
Lambda = Lambda, SigmaINV = SigmaINV, z = z)
```

```
complete.log.likelihood_q0
```

Complete log-likelihood function for xUx models and q = 0

# **Description**

Complete log-likelihood function for models with different error variance per component (xUx) and diagonal covariance structure per component (q = 0.

### Usage

```
complete.log.likelihood_q0(x_data, w, mu, SigmaINV, z)
```

# Arguments

x\_data  $n \times p$  matrix containing the data

w a vector of length K containing the mixture weights

mu  $K \times p$  matrix containing the marginal means per component

SigmaINV  $K \times p \times p$  precision matrix (inverse covariance) per component

z A vector of length n containing the allocations of the n datapoints to the K

mixture components

### Value

complete log-likelihood value

# Author(s)

```
library('fabMix')
data(waveDataset1500)
x_data <- scale(waveDataset1500[ 1:20, -1]) # data
z <- waveDataset1500[ 1:20, 1] # class
p <- dim(x_data)[2]
q <- 2
K <- length(table(z)) # 3 classes
# give some arbitrary values to the parameters:
set.seed(1)
w <- rep(1/K, K)
mu <- array( -0.1 + 0.2*runif(K * p), dim = c(K,p) )
SigmaINV <- array( 1, dim = c(K,p,p))
# compute the complete.log.likelihood ( -inf )
complete.log.likelihood_q0(x_data = x_data, w = w, mu = mu,
SigmaINV = SigmaINV, z = z)</pre>
```

```
complete.log.likelihood_q0_sameSigma  {\it Complete log-likelihood function for xCx models \ and \ q=0}
```

# Description

Complete log-likelihood function for models with same error variance per component (xCx) and diagonal covariance structure per component (q = 0.

# Usage

```
complete.log.likelihood_q0_sameSigma(x_data, w, mu, SigmaINV, z)
```

# Arguments

x\_data  $n \times p$  matrix containing the data w a vector of length K containing the mixture weights mu  $K \times p$  matrix containing the marginal means per component SigmaINV  $p \times p$  precision matrix (inverse covariance) z A vector of length n containing the allocations of the n datapoints to the K mixture components

# Value

complete log-likelihood value

### Author(s)

```
library('fabMix')
data(waveDataset1500)
x_data <- scale(waveDataset1500[ 1:20, -1]) # data
z <- waveDataset1500[ 1:20, 1] # class
p <- dim(x_data)[2]
q <- 2
K <- length(table(z)) # 3 classes
# give some arbitrary values to the parameters:
set.seed(1)
w <- rep(1/K, K)
mu <- array( -0.1 + 0.2*runif(K * p), dim = c(K,p) )
SigmaINV <- array( 1, dim = c(p,p))
# compute the complete.log.likelihood ( -inf )
complete.log.likelihood_q0_sameSigma(x_data = x_data, w = w, mu = mu,
SigmaINV = SigmaINV, z = z)</pre>
```

complete.log.likelihood\_Sj

Complete log-likelihood function for xUx models.

# Description

Complete log-likelihood function for models with different error variance per component (xUx).

### **Usage**

```
complete.log.likelihood_Sj(x_data, w, mu, Lambda, SigmaINV, z)
```

# **Arguments**

x\_data  $n \times p$  matrix containing the data w a vector of length K containing the mixture weights mu  $K \times p$  matrix containing the marginal means per component Lambda  $K \times p \times q$  array of factor loadings per component (maybe restricted to be the same) SigmaINV  $K \times p \times p$  precision matrix (inverse covariance) per component

Z

# Value

complete log-likelihood value

# Author(s)

```
library('fabMix')
data(waveDataset1500)
x_data <- waveDataset1500[ 1:20, -1] # data</pre>
z <- waveDataset1500[ 1:20, 1] # class</pre>
p \leftarrow dim(x_data)[2]
q <- 2
K <- length(table(z)) # 3 classes</pre>
# give some arbitrary values to the parameters:
set.seed(1)
w \leftarrow rep(1/K, K)
mu \leftarrow array(runif(K * p), dim = c(K,p))
Lambda <- array( runif(K*p*q), dim = c(K,p,q))
SigmaINV <- array( c(0.5, 0.75, 1), dim = c(K,p,p))
# compute the complete.log.likelihood
complete.log.likelihood_Sj(x_data = x_data, w = w, mu = mu,
Lambda = Lambda, SigmaINV = SigmaINV, z = z)
```

compute\_A\_B\_G\_D\_and\_simulate\_mu\_Lambda

Computation and simulations

### **Description**

This function simulates  $\mu$  and  $\Lambda$ .

# Usage

```
compute_A_B_G_D_and_simulate_mu_Lambda(SigmaINV,
suff_statistics, OmegaINV, K, priorConst1, T_INV, v_r)
```

# **Arguments**

SigmaINV Precision matrix  $\Sigma^{-1}$ 

suff\_statistics

 $\begin{array}{c} {\rm Sufficient\ statistics} \\ {\rm OmegaINV} & {\rm Prior\ parameter:\ } \Omega^{-1} \end{array}$ 

K Number of overfitting mixture components

 $\begin{array}{ll} {\rm priorConst1} & {\rm Prior\ constant:}\ T^{-1}\xi \\ {\rm T\_INV} & {\rm Prior\ parameter:}\ T^{-1}\xi \end{array}$ 

v\_r This vector is used to set to zero the upper right  $(q-1) \times (q-1)$  diagonal block

of factor loadings for identifiability purposes.

### Value

A list containing a draw from the conditional distributions of  $\mu$  and  $\Lambda$ :

Lambdas  $K \times p \times q$  array (factor loadings per component) mu  $K \times p$  array (marginal mean per component)

### Author(s)

Panagiotis Papastamoulis

# **Examples**

```
library('fabMix')
data(waveDataset1500)
x_data <- scale(as.matrix(waveDataset1500[ 1:20, -1])) # data</pre>
z <- waveDataset1500[ 1:20, 1] # class</pre>
p <- dim(x_data)[2]
n \leftarrow dim(x_data)[1]
q <- 2
K <- length(table(z))</pre>
                                   # 3 classes
T_{INV} \leftarrow array(data = 0, dim = c(p,p))
diag(T_INV) <- diag(var(x_data))</pre>
diag(T_INV) <- 1/diag(T_INV)</pre>
ksi <- colMeans(x_data)</pre>
priorConst1 \leftarrow array(diag(T_INV)*ksi, dim = c(p,1))
# give some arbitrary values to the parameters:
set.seed(1)
mu \leftarrow array(runif(K * p), dim = c(K,p))
y \leftarrow array(rnorm(n = q*n), dim = c(n,q))
SigmaINV <- array(data = 0, dim = c(p,p))
diag(SigmaINV) <- 0.5 + 0.5*runif(p)</pre>
OmegaINV <- diag(q)</pre>
# compute sufficient stats
suf_stat <- compute_sufficient_statistics(y = y,</pre>
 z = z, K = K, x_{data} = x_{data}
v_r < - numeric(p) #indicates the non-zero values of Lambdas
for( r in 1:p){
v_r[r] \leftarrow min(r,q)
# now simulate mu and Lambda
f2 <- compute_A_B_G_D_and_simulate_mu_Lambda(SigmaINV = SigmaINV,
                 suff_statistics = suf_stat, OmegaINV = OmegaINV,
                 K = K, priorConst1 = priorConst1, T_INV = T_INV, v_r = v_r)
# f2$mu contains the simulated means
# f2$Lambdas contains the simulated factor loadings
```

```
\label{lem:compute_ABGD_and_simulate_mu_Lambda_CCU} Computation\ and\ simulations\ for\ CCU
```

# **Description**

This function simulates  $\mu$  and  $\Lambda$  for the CCU model.

### Usage

```
compute_A_B_G_D_and_simulate_mu_Lambda_CCU(SigmaINV,
suff_statistics, OmegaINV, K, priorConst1, T_INV, v_r)
```

### **Arguments**

 $\begin{array}{ll} {\rm SigmaINV} & {\rm Precision~matrix~} \Sigma^{-1} \\ {\rm suff\_statistics} & {\rm Sufficient~statistics} \\ {\rm OmegaINV} & {\rm Prior~parameter:~} \Omega^{-1} \end{array}$ 

K Number of overfitting mixture components

 $\begin{array}{ll} {\rm priorConst1} & {\rm Prior\ constant:}\ T^{-1}\xi \\ {\rm T\_INV} & {\rm Prior\ parameter:}\ T^{-1}\xi \end{array}$ 

v\_r This vector is used to set to zero the upper right  $(q-1) \times (q-1)$  diagonal block

of factor loadings for identifiability purposes.

### Value

A list containing a draw from the conditional distributions of  $\mu$  and  $\Lambda$ :

Lambdas  $K \times p \times q$  array (factor loadings per component) mu  $K \times p$  array (marginal mean per component)

### Author(s)

Panagiotis Papastamoulis

# **Examples**

```
library('fabMix')
data(waveDataset1500)
x_data <- scale(as.matrix(waveDataset1500[ 1:20, -1])) # data</pre>
z <- waveDataset1500[ 1:20, 1] # class</pre>
p <- dim(x_data)[2]
n <- dim(x_data)[1]
q <- 2
K <- length(table(z))</pre>
                                   # 3 classes
# give some arbitrary values to the parameters:
set.seed(1)
mu \leftarrow array(runif(K * p), dim = c(K,p))
y \leftarrow array(rnorm(n = q*n), dim = c(n,q))
SigmaINV <- array(data = 0, dim = c(p,p))
diag(SigmaINV) = 0.5 + 0.5*runif(p)
OmegaINV <- diag(q)</pre>
# compute sufficient stats
suf_stat <- compute_sufficient_statistics_given_mu(y = y,</pre>
z = z, K = K, x_{data} = x_{data}, mu = mu)
v_r \leftarrow numeric(p) #indicates the non-zero values of Lambdas
```

```
\label{lem:compute_ABGD_and_simulate_mu_Lambda_CUU} Computation\ and\ simulations\ for\ CUU
```

# **Description**

This function simulates  $\mu$  and  $\Lambda$  for the CUU model.

# Usage

```
compute_A_B_G_D_and_simulate_mu_Lambda_CUU(SigmaINV,
suff_statistics, OmegaINV, K, priorConst1, T_INV, v_r)
```

# **Arguments**

 $\begin{array}{ll} {\rm SigmaINV} & {\rm Precision~matrix~} \Sigma^{-1} \\ {\rm suff\_statistics} \end{array}$ 

K Number of overfitting mixture components

priorConst1 Prior constant:  $T^{-1}\xi$ T\_INV Prior parameter:  $T^{-1}\xi$ 

v\_r This vector is used to set to zero the upper right  $(q-1) \times (q-1)$  diagonal block

of factor loadings for identifiability purposes.

### Value

A list containing a draw from the conditional distributions of  $\mu$  and  $\Lambda$ :

Lambdas  $K \times p \times q$  array (factor loadings per component) mu  $K \times p$  array (marginal mean per component)

### Author(s)

Panagiotis Papastamoulis

# **Examples**

```
library('fabMix')
data(waveDataset1500)
x_data <- scale(as.matrix(waveDataset1500[ 1:20, -1])) # data</pre>
z <- waveDataset1500[ 1:20, 1] # class</pre>
p <- dim(x_data)[2]
n \leftarrow dim(x_data)[1]
q <- 2
                                   # 3 classes
K <- length(table(z))</pre>
# give some arbitrary values to the parameters:
set.seed(1)
mu \leftarrow array(runif(K * p), dim = c(K,p))
y \leftarrow array(rnorm(n = q*n), dim = c(n,q))
SigmaINV \leftarrow array(data = 0, dim = c(K,p,p))
for(k in 1:K){
diag(SigmaINV[k,,]) \leftarrow 0.5 + 0.5*runif(p)
OmegaINV <- diag(q)</pre>
# compute sufficient stats
suf_stat <- compute_sufficient_statistics_given_mu(y = y,</pre>
z = z, K = K, x_{data} = x_{data}, mu = mu)
v_r <- numeric(p) #indicates the non-zero values of Lambdas</pre>
for( r in 1:p ){
v_r[r] \leftarrow min(r,q)
T_{INV} \leftarrow array(data = 0, dim = c(p,p))
diag(T_INV) <- diag(var(x_data))</pre>
diag(T_INV) <- 1/diag(T_INV)</pre>
ksi <- colMeans(x_data)</pre>
priorConst1 <- array(diag(T_INV)*ksi, dim =c(p,1))</pre>
# now simulate mu and Lambda
f2 <- compute_A_B_G_D_and_simulate_mu_Lambda_CUU(SigmaINV = SigmaINV,</pre>
                 suff_statistics = suf_stat, OmegaINV = OmegaINV,
                 K = K, priorConst1 = priorConst1, T_INV = T_INV, v_r = v_r)
# f2$mu contains the simulated means
# f2$Lambdas contains the simulated factor loadings
```

```
\label{eq:compute_ABGD_and_simulate_mu_Lambda_q0} Computation\ and\ simulations\ for\ q=0.
```

# **Description**

This function simulates  $\mu$ .

### Usage

```
compute_A_B_G_D_and_simulate_mu_Lambda_q0(SigmaINV,
suff_statistics, K, priorConst1, T_INV, v_r)
```

# **Arguments**

SigmaINV Precision matrix  $\Sigma^{-1}$ 

suff\_statistics

Sufficient statistics

K Number of overfitting mixture components

priorConst1 Prior constant:  $T^{-1}\xi$ T\_INV Prior parameter:  $T^{-1}\xi$ 

v\_r This vector is used to set to zero the upper right  $(q-1) \times (q-1)$  diagonal block

of factor loadings for identifiability purposes.

### Value

A list containing a draw from the conditional distributions of  $\mu$ :

mu  $K \times p$  array (marginal mean per component)

### Author(s)

Panagiotis Papastamoulis

```
\label{lem:compute_A_B_G_D_and_simulate_mu_Lambda_q0_sameSigma} Computation\ and\ simulations\ for\ q=0.
```

# Description

This function simulates  $\mu$ .

# Usage

```
\label{lem:compute_A_B_G_D_and_simulate_mu_Lambda_q0_sameSigma(SigmaINV, suff_statistics, K, priorConst1, T_INV, v_r)
```

# **Arguments**

SigmaINV Precision matrix  $\Sigma^{-1}$ 

suff\_statistics

Sufficient statistics

K Number of overfitting mixture components

 $\begin{array}{ll} {\rm priorConst1} & {\rm Prior\ constant:}\ T^{-1}\xi \\ {\rm T\_INV} & {\rm Prior\ parameter:}\ T^{-1}\xi \end{array}$ 

v\_r This vector is used to set to zero the upper right  $(q-1) \times (q-1)$  diagonal block

of factor loadings for identifiability purposes.

### Value

A list containing a draw from the conditional distributions of  $\mu$ :

mu  $K \times p$  array (marginal mean per component)

### Author(s)

Panagiotis Papastamoulis

# Description

This function simulates  $\mu$  and  $\Lambda$ .

# Usage

```
compute_A_B_G_D_and_simulate_mu_Lambda_Sj(SigmaINV,
suff_statistics, OmegaINV, K, priorConst1, T_INV, v_r)
```

### **Arguments**

SigmaINV Precision matrix  $\Sigma^{-1}$  per component

suff\_statistics

Sufficient statistics

OmegaINV Prior parameter:  $\Omega^{-1}$ 

K Number of overfitting mixture components

 $\begin{array}{ll} {\rm priorConst1} & {\rm Prior\ constant:}\ T^{-1}\xi \\ {\rm T\_INV} & {\rm Prior\ parameter:}\ T^{-1}\xi \end{array}$ 

v\_r This vector is used to set to zero the upper right  $(q-1) \times (q-1)$  diagonal block

of factor loadings for identifiability purposes.

### Value

A list containing a draw from the conditional distributions of  $\mu$  and  $\Lambda$ :

Lambdas  $K \times p \times q$  array (factor loadings per component) mu  $K \times p$  array (marginal mean per component)

# Author(s)

```
library('fabMix')
data(waveDataset1500)
x_data <- scale(as.matrix(waveDataset1500[ 1:20, -1])) # data</pre>
z <- waveDataset1500[ 1:20, 1] # class</pre>
p <- dim(x_data)[2]</pre>
n \leftarrow dim(x_data)[1]
q <- 2
K <- length(table(z))</pre>
                                   # 3 classes
# give some arbitrary values to the parameters:
set.seed(1)
mu <- array( runif(K * p), dim = c(K,p) )
y \leftarrow array(rnorm(n = q*n), dim = c(n,q))
SigmaINV <- array(data = 0, dim = c(K,p,p))
for(k in 1:K){
diag(SigmaINV[k,,]) \leftarrow 0.5 + 0.5*runif(p)
OmegaINV <- diag(q)</pre>
# compute sufficient stats
suf_stat <- compute_sufficient_statistics(y = y,</pre>
z = z, K = K, x_{data} = x_{data}
v_r <- numeric(p) #indicates the non-zero values of Lambdas</pre>
for( r in 1:p ){
v_r[r] \leftarrow min(r,q)
}
T_{INV} \leftarrow array(data = 0, dim = c(p,p))
diag(T_INV) <- diag(var(x_data))</pre>
diag(T_INV) <- 1/diag(T_INV)</pre>
ksi <- colMeans(x_data)</pre>
priorConst1 <- array(diag(T_INV)*ksi, dim =c(p,1))</pre>
# now simulate mu and Lambda
f2 <- compute_A_B_G_D_and_simulate_mu_Lambda_Sj(SigmaINV = SigmaINV,</pre>
                 suff_statistics = suf_stat, OmegaINV = OmegaINV,
                 K = K, priorConst1 = priorConst1, T_INV = T_INV, v_r = v_r)
# f2$mu contains the simulated means
# f2$Lambdas contains the simulated factor loadings
```

compute\_sufficient\_statistics

Compute sufficient statistics

### **Description**

Compute sufficient statistics given y and z.

# Usage

```
compute_sufficient_statistics(y, z, K, x_data)
```

# **Arguments**

у	$n \times q$ matrix of factors
Z	Allocation vector
K	Number of components
x data	$n \times p$ matrix with observed data

# Value

A list with six entries of sufficient statistics.

cluster_size	Integer vector of length $K$
sx	$K \times p$ array
sy	$K \times q$ array
sxx	Not used
syy	$K \times q \times q$ array
sxy	$K \times p \times q$ array

# Author(s)

Panagiotis Papastamoulis

# **Examples**

```
data(waveDataset1500)
    x_data <- as.matrix(waveDataset1500[ 1:20, -1]) # data
    z <- waveDataset1500[ 1:20, 1] # class
    p <- dim(x_data)[2]
    n <- dim(x_data)[1]
    q <- 2
    K <- length(table(z)) # 3 classes
    # give some arbitrary values to the parameters:
    set.seed(1)
y <- array(rnorm(n = q*n), dim = c(n,q))
# compute sufficient stats
suf_stat <- compute_sufficient_statistics(y = y,
    z = z, K = K, x_data = x_data)</pre>
```

```
compute_sufficient_statistics_given_mu

Compute sufficient statistics given mu
```

# Description

Compute sufficient statistics given y, z and  $\mu$ .

# Usage

```
compute_sufficient_statistics_given_mu(y, z, K, x_data,mu)
```

# **Arguments**

у	$n \times q$ matrix of factors
z	Allocation vector
K	Number of components
x_data	$n \times p$ matrix with observed data
mu	$K \times p$ matrix with marignal means per component

### Value

A list with six entries of sufficient statistics.

cluster_size	Integer vector of length K
sx	$K \times p$ array
sy	$K \times q$ array
sxx	Not used
syy	$K \times q \times q$ array
sxy	$K \times p \times q$ array

# Author(s)

Panagiotis Papastamoulis

# **Examples**

```
data(waveDataset1500)
    x_data <- as.matrix(waveDataset1500[ 1:20, -1]) # data
    z <- waveDataset1500[ 1:20, 1] # class
    p <- dim(x_data)[2]
    n <- dim(x_data)[1]
    q <- 2
    K <- length(table(z)) # 3 classes
    # give some arbitrary values to the parameters:
    set.seed(1)
    mu <- array( runif(K * p), dim = c(K,p) )
y <- array(rnorm(n = q*n), dim = c(n,q))
# compute sufficient stats
suf_stat <- compute_sufficient_statistics_given_mu(y = y,
    z = z, K = K, x_data = x_data, mu = mu)</pre>
```

```
\label{eq:compute_sufficient_statistics_q0} \textit{Compute sufficient statistics for } q = 0
```

# Description

Compute sufficient statistics given z.

# Usage

```
compute_sufficient_statistics_q0(z, K, x_data)
```

# **Arguments**

Z	Allocation vector
K	Number of components
x_data	Data

### Value

A list with six entries of sufficient statistics.

cluster_size	Integer vector of length K
sx	$K \times p$ array
sy	Not used here
SXX	Not used
syy	Not used here
sxy	Not used here

### Author(s)

Panagiotis Papastamoulis

# **Examples**

```
\label{eq:data} $\operatorname{data}(\operatorname{waveDataset1500})$ \\ x_{data} <- \operatorname{as.matrix}(\operatorname{waveDataset1500}[\ 1:20,\ -1]) \ \# \ \operatorname{data} \\ z <- \operatorname{waveDataset1500}[\ 1:20,\ 1] \ \# \ \operatorname{class} \\ p <- \operatorname{dim}(x_{data})[2] \\ n <- \operatorname{dim}(x_{data})[1] \\ q <- 2 \\ K <- \operatorname{length}(\operatorname{table}(z)) \ \# \ 3 \ \operatorname{classes} \\ \# \ \operatorname{compute} \ \operatorname{sufficient} \ \operatorname{stats} \\ \operatorname{suf\_stat} <- \operatorname{compute\_sufficient\_statistics\_q0}( \\ z = z, \ K = K, \ x_{data} = x_{data}) \\
```

CorMat\_mcmc\_summary

Compute quantiles for the correlation matrix.

# Description

Compute quantiles for the correlation matrix per cluster based on the MCMC output stored in a fabMix.object.

# Usage

```
CorMat_mcmc_summary(x, quantile_probs)
```

# **Arguments**

x An object of class fabMix.object.

quantile\_probs Vector of probabilities for computing the corresponding quantiles.

# Value

quantiles A list containing the quantiles for the correlation matrix per component. Each

element is a  $p \times p \times K$  array, where p and K denote the dimension of the multivariate data and number of alive components for the selected model, re-

spectively.

p\_matrix A  $p \times p \times K$  array, where for each k = 1, ..., K the  $p \times p$  matrix p\_matrix[,,k]

contains the posterior probability  $1 - 2|0.5 - P(\rho_{ij} > 0)|$  for  $i = 1, \dots, p$ ;

 $j=1,\ldots,p.$ 

### Author(s)

Panagiotis Papastamoulis

CovMat\_mcmc\_summary

Compute quantiles for the covariance matrix.

### **Description**

Compute quantiles for the covariance matrix per cluster based on the MCMC output stored in a fabMix.object.

# Usage

```
CovMat_mcmc_summary(x, quantile_probs)
```

# Arguments

```
x An object of class fabMix.object.
quantile_probs Vector of probabilities for computing the corresponding quantiles.
```

### Value

A list containing the quantiles for the covariance matrix per component. Each element is a  $p \times p \times K$  array, where p and K denote the dimension of the multivariate data and number of alive components for the selected model, respectively.

### Author(s)

Panagiotis Papastamoulis

dealWithLabelSwitching

Apply label switching algorithms

# **Description**

This functions is a wrapper for the label. switching package and applies the ECR and ECR.ITERATIVE.1 algorithms. The model may have the same variance of error terms per cluster or not.

### Usage

```
dealWithLabelSwitching(sameSigma, x_data, outputFolder, q, burn,
z.true, compute_regularized_expression, Km)
```

# Arguments

sameSigma Logical value indicating whether the parameterization with the same error vari-

ance per cluster is used.

x\_data Data

outputFolder Name of the folder where the fabMix function has saved its output

q Number of factors

burn Discard observations as burn-in period (optional).

z.true An (optional) vector of cluster assignments which is considered as the groun-

truth clustering of the data. Useful for direct comparisons against the real pa-

rameter values in simulated data.

compute\_regularized\_expression

Logical. Should regularized expression be computed?

Km Number of components in the overfitted mixture model.

### Value

The following files are produced in the output folder:

### Author(s)

Panagiotis Papastamoulis

### References

Papastamoulis, P. (2016). label.switching: An R Package for Dealing with the Label Switching Problem in MCMC Outputs. Journal of Statistical Software, 69(1), 1-24.

	fabMix	Main function		
--	--------	---------------	--	--

# **Description**

This function runs parallel chains under a prior tempering scheme of the Dirichlet prior distribution of mixture weights.

# Usage

```
fabMix(model, nChains, dirPriorAlphas, rawData, outDir, Kmax, mCycles,
burnCycles, g, h, alpha_sigma, beta_sigma, q, normalize,
thinning, zStart, nIterPerCycle, gibbs_z,
warm_up_overfitting, warm_up, overfittingInitialization,
progressGraphs, gwar, rmDir, parallelModels)
```

# **Arguments**

model	Any subset of "UUU" "CUU" "UCU" "CCU" "UCC" "UUC" "CUC", "CCC" indicating the fitted models. By default, all models are fitted.
nChains	The number of parallel heated chains. When 'dirPriorAlphas' is supplied, 'nChains' can be ignored.
dirPriorAlphas	vector of length nChains in the form of an increasing sequence of positive scalars. Each entry contains the (common) prior Dirichlet parameter for the corresponding chain. Default: dirPriorAlphas = $c(1, 1 + dN*(2:nChains - 1))/Kmax$ , where $dN = 1$ , for nChains > 1. Otherwise, dirPriorAlphas = $1/Kmax$ .
rawData	The observed data as an $n \times p$ matrix. Clustering is performed on the rows of the matrix.
outDir	Name of the output folder. An error is thrown if the directory already exists inside the current working directory. Note: it should NOT correspond to an absolute path, e.g.: outDir = `fabMix_example` is acceptable, but outDir = `C:\Username\Documents\fabMix_example` is not.
Kmax	Number of components in the overfitted mixture. Default: 20.
mCycles	Number of MCMC cycles. Each cycle consists of nIterPerCycle MCMC iterations. At the end of each cycle a swap of the state of two randomly chosen adjacent chains is attempted.
burnCycles	Number of cycles that will be discarded as burn-in period.

g Prior parameter g. Default value: g=0.5. h Prior parameter h. Default value: h=0.5. alpha\_sigma Prior parameter  $\alpha$ . Default value:  $\alpha=0.5$ . beta\_sigma Prior parameter  $\beta$ . Default value:  $\beta=0.5$ .

q A vector containing the number of factors to be fitted.

normalize Should the observed data be normalized? Default value: TRUE. (Recommended)

thinning Optional integer denoting the thinning of the keeped MCMC cycles.

zStart Optional starting value for the allocation vector.

nIterPerCycle Number of iteration per MCMC cycle. Default value: 10.

gibbs\_z Select the gibbs sampling scheme for updating latent allocations of mixture

model. Default value: 1.

warm\_up\_overfitting

Number of iterations for the overfitting initialization scheme. Default value:

500.

warm\_up Number of iterations that will be used to initialize the models before starting

proposing switchings. Default value: 5000.

overfittingInitialization

Logical value indicating whether the chains are initialized via the overfitting

initialization scheme. Default: TRUE.

progressGraphs Logical value indicating whether to plot successive states of the chains while the

sampler runs. Default: FALSE.

gwar Initialization parameter. Default: 0.05.

rmDir Logical value indicating whether to delete the outDir directory. Default: TRUE.

parallelModels Model-level parallelization: An optional integer specifying the number of cores

that will be used in order to fit in parallel each member of model. Default:

NULL (no model-level parallelization).

# **Details**

Let  $X_i$ ;  $i=1,\ldots,n$  denote independent p-dimensional random vectors. Let  $Y_i \in R^q$  with q < p denote the latent factor for observation  $i=1,\ldots,n$ . In the typical factor analysis model, each observation is modelled as  $X_i = \mu + \Lambda Y_i + \varepsilon_i$ , with  $\varepsilon_i \sim \mathcal{N}(0,\Sigma)$ , where  $\varepsilon_i$  and  $Y_i$  are assumed independent,  $i=1,\ldots,n$ . The  $p \times q$  matrix  $\Lambda$  consists of the factor loadings. Assume that there are K clusters and let  $Z_i$  denotes the latent allocation of observation i to one amongs the k clusters, with prior probability  $P(Z_i = k) = w_k, k = 1,\ldots,K$ , independent for  $i=1,\ldots,n$ . Following McNicholas et al (2008), the following parameterizations are used:

UUU model:  $(\boldsymbol{X}_i|Z_i=k)=\boldsymbol{\mu}_k+\boldsymbol{\Lambda}_k\boldsymbol{Y}_i+\boldsymbol{\varepsilon}_i, \text{ with }\boldsymbol{\varepsilon}_i\sim\mathcal{N}(0,\boldsymbol{\Sigma}_k)$ UCU model:  $(\boldsymbol{X}_i|Z_i=k)=\boldsymbol{\mu}_k+\boldsymbol{\Lambda}_k\boldsymbol{Y}_i+\boldsymbol{\varepsilon}_i, \text{ with }\boldsymbol{\varepsilon}_i\sim\mathcal{N}(0,\boldsymbol{\Sigma})$ UUC model:  $(\boldsymbol{X}_i|Z_i=k)=\boldsymbol{\mu}_k+\boldsymbol{\Lambda}_k\boldsymbol{Y}_i+\boldsymbol{\varepsilon}_i, \text{ with }\boldsymbol{\varepsilon}_i\sim\mathcal{N}(0,\sigma_k\boldsymbol{I}_p)$ UCC model:  $(\boldsymbol{X}_i|Z_i=k)=\boldsymbol{\mu}_k+\boldsymbol{\Lambda}_k\boldsymbol{Y}_i+\boldsymbol{\varepsilon}_i, \text{ with }\boldsymbol{\varepsilon}_i\sim\mathcal{N}(0,\sigma\boldsymbol{I}_p)$ CUU model:  $(\boldsymbol{X}_i|Z_i=k)=\boldsymbol{\mu}_k+\boldsymbol{\Lambda}\boldsymbol{Y}_i+\boldsymbol{\varepsilon}_i, \text{ with }\boldsymbol{\varepsilon}_i\sim\mathcal{N}(0,\boldsymbol{\Sigma}_k)$ CCU model:  $(\boldsymbol{X}_i|Z_i=k)=\boldsymbol{\mu}_k+\boldsymbol{\Lambda}\boldsymbol{Y}_i+\boldsymbol{\varepsilon}_i, \text{ with }\boldsymbol{\varepsilon}_i\sim\mathcal{N}(0,\boldsymbol{\Sigma}_k)$ 

CUC model:  $(X_i|Z_i = k) = \mu_k + \Lambda Y_i + \varepsilon_i$ , with  $\varepsilon_i \sim \mathcal{N}(0, \sigma_k I_p)$ CCC model:  $(X_i|Z_i = k) = \mu_k + \Lambda Y_i + \varepsilon_i$ , with  $\varepsilon_i \sim \mathcal{N}(0, \sigma I_p)$ 

In all cases,  $\varepsilon_i$  and  $Y_i$  are assumed independent,  $i=1,\ldots,n$ . Note that  $\Sigma_k$  and  $\Sigma$  denote positive definite matrices,  $I_p$  denotes the  $p \times p$  identity matrix and  $\sigma_k$ ,  $\sigma$  denote positive scalars.

### Value

An object of class fabMix.object, that is, a list consisting of the following entries:

bic Bayesian Information Criterion per model and number of factors.

class The estimated single best clustering of the observations according to the selected

model.

n\_Clusters\_per\_model

The most probable number of clusters (number of non-empty components of the

overfitted mixture) per model and number of factors.

posterior\_probability

The posterior probability of the estimated allocations according to the selected

model.

covariance\_matrix

The estimated posterior mean of the covariance matrix per cluster according to

the selected model.

mu The estimated posterior mean of the mean per cluster according to the selected

model.

weights The estimated posterior mean of the mixing proportions according to the se-

lected model.

selected\_model

Data frame containing the parameterization, number of clusters and factors of

the selected model.

mcmc A list containing the MCMC draws for the parameters of the selected model.

Each entry is returned as an mcmc object, a class imported from the coda package (Plummer et al, 2006). All component-specific parameters have been reordered according to the ECR algorithm in order to undo the label switching problem. However, the output corresponding to factor scores and factor loadings is not

identifiable due to sign-switching across the MCMC trace.

data The observed data.

regularizedExpression

The regularized expressions of variable scores to each factor per cluster (see

Papastamoulis 2018, CSDA).

Kmap\_prob The posterior probability of the Maximum A Posterior number of alive clusters

for each parameterization and factor level.

### Note

It is recommended to use: normalize = TRUE (default). Tuning of dirPriorAlphas may be necessary to achieve reasonable acceptance rates of chain swaps. Note that the output is reordered in order to deal with the label switching problem, according to the ECR algorithm applied by dealWithLabelSwitching function.

Parallelization is enabled in both the chain-level as well as the model-level. By default all heated chains (specified by the nchains argument) run in parallel using (at most) the same number of threads (if available). If parallelModels = NULL (default), then the selected parameterizations will run (serially) on the same thread. Otherwise, if parallelModels = x (where x denotes a positive integer), the algorithm will first use x threads to fit the specified model parameterizations in parallel, and furthermore will also parallelize the heated chains (according to the remaining free cores on the user's system). The user should combine parallelModels with nChains efficiently, for example: if the number of available threads equals 12 and the user wishes to run 3 heated chains per model (recall that there are 8 parameterizations in total), then, an ideal allocation would be parallelModels = 4 and nChains = 3 because all available threads will be constantly busy. If the user wishes to run nChains = 4 heated chains per model using 12 threads, then an ideal allocation would be parallelModels = 3 models running in parallel. In the case where parallelModels\*nChains > m, with m denoting the available number of threads, the algorithm will first allocate min(parallelModels, m) threads to run the same number of parameterizations in parallel, and then the remaining threads (if any) will be used to process the parallel heated chains. If no other threads are available, the heated chains will be allocated to single threads.

#### Author(s)

Panagiotis Papastamoulis

#### References

Martyn Plummer, Nicky Best, Kate Cowles and Karen Vines (2006). CODA: Convergence Diagnosis and Output Analysis for MCMC, R News, vol 6, 7-11.

McNicholas, P.D. and Murphy, T.B. Stat Comput (2008) 18: 285. https://doi.org/10.1007/s11222-008-9056-0.

Papastamoulis, P. (2018). Overfitting Bayesian mixtures of factor analyzers with an unknown number of components. Computational Statistics and Data Analysis, 124: 220-234. DOI: 10.1016/j.csda.2018.03.007.

### See Also

```
plot.fabMix.object
```

### **Examples**

```
syntheticDataset <- simData(sameLambda=TRUE,K.true = K, n = n, q = q, p = p,
sINV_values = sINV_diag)
colnames(syntheticDataset$data) <- paste0("x_",1:p)</pre>
# Run `fabMix` for a _small_ number of iterations for the
# `UUU` (maximal model) and `CCC` (minimal model) parameterizations,
# using the default prior parallel heating parameters `dirPriorAlphas`.
# NOTE: `dirPriorAlphas` may require some tuning in general.
qRange <- 2 \# values for the number of factors (only the true number
                                                 is considered here)
Kmax <- 4 # number of components for the overfitted mixture model
nChains <- 2 # number of parallel heated chains
set.seed(1)
fm <- fabMix( model = c("UUU", "CCC"), nChains = nChains,</pre>
rawData = syntheticDataset$data, outDir = "toyExample",
       Kmax = Kmax, mCycles = 4, burnCycles = 1, q = qRange,
       g = 0.5, h = 0.5, alpha_sigma = 0.5, beta_sigma = 0.5,
       warm_up_overfitting = 2, warm_up = 5)
# WARNING: the following parameters:
# Kmax, nChains, mCycles, burnCycles, warm_up_overfitting, warm_up
# should take (much) _larger_ values. E.g. a typical implementation consists of:
#
        Kmax = 20, nChains >= 3, mCycles = 1100, burnCycles = 100,
        warm_up_overfitting = 500, warm_up = 5000.
# You may also print and plot
# print(fm)
# plot(fm, what = "BIC")
# (b) using 12 cores______
#_____4 models with 3 heated chains running in parallel_____
#_____considering all 8 model parameterizations_____
## Not run:
library('fabMix')
set.seed(99)
                     # sample size
n = 200
p = 30
                    # number of variables
q = 2
                   # number of factors
K = 5 # number of clusters
sINV_diag = rep(1/20,p) # diagonal of inverse variance of errors
syntheticDataset <- simData(sameLambda=FALSE,K.true = K, n = n, q = q, p = p,
sINV_values = sINV_diag)
colnames(syntheticDataset$data) <- paste0("x_",1:p)</pre>
qRange <- 1:3 # range of values for the number of factors
Kmax <- 20 # number of components for the overfitted mixture model
nChains <- 3 # number of parallel heated chains
# the next command takes \sim 2 hours in a Linux machine with 12 threads.
```

28 fabMix\_CxC

fabMix\_CxC

Function to estimate the CUC and CCC models

# **Description**

This function runs parallel chains under a prior tempering scheme of the Dirichlet prior distribution of mixture weights.

# Usage

```
fabMix_CxC(sameSigma, dirPriorAlphas, rawData, outDir, Kmax, mCycles,
burnCycles, g, h, alpha_sigma, beta_sigma, q, normalize,
thinning, zStart, nIterPerCycle, gibbs_z,
warm_up_overfitting, warm_up, overfittingInitialization,
progressGraphs, gwar, cccStart)
```

# **Arguments**

sameSigma Logical value denoting the parameterization of the error variance per compo-

nent. If TRUE, the parameterization CCU is fitted. Otherwise, the parameteriza-

tion CUU is fitted.

dirPriorAlphas The prior Dirichlet parameters for each chain.

rawData The observed data as an  $n \times p$  matrix. Clustering is performed on the rows of

the matrix.

outDir Name of the output folder.

Kmax Number of components in the overfitted mixture. Default: 20.

mCycles Number of MCMC cycles. Each cycle consists of nIterPerCycle MCMC it-

erations. At the end of each cycle a swap of the state of two randomly chosen

adjacent chains is attempted.

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burnCycles Number of cycles that will be discarded as burn-in period.

g Prior parameter g. Default value: g=2. h Prior parameter h. Default value: h=1. alpha\_sigma Prior parameter  $\alpha$ . Default value:  $\alpha=2$ . beta\_sigma Prior parameter  $\beta$ . Default value:  $\beta=1$ .

Number of factors q, where  $1 \le q \le L$ . An error is thrown if the Ledermann

bound (L) is exceeded.

normalize Should the observed data be normalized? Default value: TRUE. thinning Optional integer denoting the thinning of the keeped MCMC cycles.

zStart Optional starting value for the allocation vector.

nIterPerCycle Number of iteration per MCMC cycle. Default value: 10.

gibbs\_z Select the gibbs sampling scheme for updating latent allocations of mixture

model. Default value: 1.

warm\_up\_overfitting

Number of iterations for the overfitting initialization scheme. Default value:

100.

warm\_up Number of iterations that will be used to initialize the models before starting

proposing switchings. Default value: 500.

overfittingInitialization

Logical value indicating whether the chains are initialized via the overfitting

initialization scheme. Default: TRUE.

progressGraphs Logical value indicating whether to plot successive states of the chains while the

sampler runs. Default: FALSE.

gwar Initialization parameter. Default: 0.05. cccStart Initialization from the CCC model.

### Value

List of files written to outDir

# Note

It is recommended to always use: normalize = TRUE (default). Tuning of dirPriorAlphas may be necessary to achieve reasonable acceptance rates of chain swaps. Also note that the output is not identifiable due to label switching and the user has to subsequently call the dealWithLabelSwitching function. See the fabMix function for examples.

### Author(s)

Panagiotis Papastamoulis

### See Also

fabMix

30 fabMix\_CxU

# **Description**

This function runs parallel chains under a prior tempering scheme of the Dirichlet prior distribution of mixture weights.

### **Usage**

```
fabMix_CxU(sameSigma, dirPriorAlphas, rawData, outDir, Kmax, mCycles,
burnCycles, g, h, alpha_sigma, beta_sigma, q, normalize,
thinning, zStart, nIterPerCycle, gibbs_z,
warm_up_overfitting, warm_up, overfittingInitialization,
progressGraphs, gwar)
```

### **Arguments**

sameSigma Logical value denoting the parameterization of the error variance per compo-

nent. If TRUE, the parameterization CCU is fitted. Otherwise, the parameteriza-

tion CUU is fitted.

dirPriorAlphas The prior Dirichlet parameters for each chain.

rawData The observed data as an  $n \times p$  matrix. Clustering is performed on the rows of

the matrix.

outDir Name of the output folder.

Kmax Number of components in the overfitted mixture. Default: 20.

mCycles Number of MCMC cycles. Each cycle consists of nIterPerCycle MCMC it-

erations. At the end of each cycle a swap of the state of two randomly chosen

adjacent chains is attempted.

burnCycles Number of cycles that will be discarded as burn-in period.

g Prior parameter g. Default value: g=2. h Prior parameter h. Default value: h=1. alpha\_sigma Prior parameter  $\alpha$ . Default value:  $\alpha=2$ . beta\_sigma Prior parameter  $\beta$ . Default value:  $\beta=1$ .

Number of factors q, where  $1 \le q \le L$ . An error is thrown if the Ledermann

bound (L) is exceeded.

normalize Should the observed data be normalized? Default value: TRUE. thinning Optional integer denoting the thinning of the keeped MCMC cycles.

zStart Optional starting value for the allocation vector.

nIterPerCycle Number of iteration per MCMC cycle. Default value: 10.

gibbs\_z Select the gibbs sampling scheme for updating latent allocations of mixture

model. Default value: 1.

warm\_up\_overfitting

Number of iterations for the overfitting initialization scheme. Default value:

100.

warm\_up Number of iterations that will be used to initialize the models before starting

proposing switchings. Default value: 500.

overfittingInitialization

Logical value indicating whether the chains are initialized via the overfitting

initialization scheme. Default: TRUE.

progressGraphs Logical value indicating whether to plot successive states of the chains while the

sampler runs. Default: FALSE.

gwar Initialization parameter. Default: 0.05.

#### Value

List of files written to outDir

### Note

It is recommended to always use: normalize = TRUE (default). Tuning of dirPriorAlphas may be necessary to achieve reasonable acceptance rates of chain swaps. Also note that the output is not identifiable due to label switching and the user has to subsequently call the dealWithLabelSwitching function. See the fabMix function for examples.

### Author(s)

Panagiotis Papastamoulis

# See Also

fabMix

fabMix\_missing\_values Function to estimate the UUU or UCU models in case of missing values

### **Description**

This function runs parallel chains under a prior tempering scheme of the Dirichlet prior distribution of mixture weights. Missing values are simulated from their full conditional posterior distribution.

### Usage

```
fabMix_missing_values(sameSigma, dirPriorAlphas, rawData, outDir, Kmax, mCycles,
burnCycles, g, h, alpha_sigma, beta_sigma, q, normalize,
thinning, zStart, nIterPerCycle, gibbs_z, warm_up,
progressGraphs, gwar)
```

### **Arguments**

sameSigma Logical value denoting the parameterization of the error variance per compo-

nent. If sameSigma = TRUE, the parameterization UCU is fitted, otherwise the

UUU model is fitted.

dirPriorAlphas The prior Dirichlet parameters for each chain.

rawData The observed data as an  $n \times p$  matrix. Clustering is performed on the rows of

the matrix.

outDir Name of the output folder.

Kmax Number of components in the overfitted mixture. Default: 20.

mCycles Number of MCMC cycles. Each cycle consists of nIterPerCycle MCMC it-

erations. At the end of each cycle a swap of the state of two randomly chosen

adjacent chains is attempted.

burnCycles Number of cycles that will be discarded as burn-in period.

g Prior parameter g. Default value: g=2. h Prior parameter h. Default value: h=1. alpha\_sigma Prior parameter  $\alpha$ . Default value:  $\alpha=2$ . beta\_sigma Prior parameter  $\beta$ . Default value:  $\beta=1$ .

q Number of factors q, where  $1 \le q \le L$ . An error is thrown if the Ledermann

bound (L) is exceeded.

normalize Should the observed data be normalized? Default value: TRUE. thinning Optional integer denoting the thinning of the keeped MCMC cycles.

zStart Optional starting value for the allocation vector.

nIterPerCycle Number of iteration per MCMC cycle. Default value: 10.

gibbs\_z Select the gibbs sampling scheme for updating latent allocations of mixture

model. Default value: 1.

warm\_up NUmber of iterations that will be used to initialize the models before starting

proposing switchings. Default value: 500.

progressGraphs Logical value indicating whether to plot successive states of the chains while the

sampler runs. Default: FALSE.

gwar Initialization parameter. Default: 0.05.

### Value

List of files written to outDir

#### Note

It is recommended to always use: normalize = TRUE (default). Tuning of dirPriorAlphas may be necessary to achieve reasonable acceptance rates of chain swaps. Also note that the output is not identifiable due to label switching and the user has to subsequently call the dealWithLabelSwitching function.

### Author(s)

 ${\tt fabMix\_parallelModels} \ \ \textit{Function for model-level parallelization}$ 

# **Description**

This function runs multiple copies of the fabMix function in parallel.

# Usage

```
fabMix_parallelModels(model, nChains, dirPriorAlphas, rawData, outDir, Kmax, mCycles,
burnCycles, g, h, alpha_sigma, beta_sigma, q, normalize,
thinning, zStart, nIterPerCycle, gibbs_z,
warm_up_overfitting, warm_up, overfittingInitialization,
progressGraphs, gwar, rmDir, parallelModels)
```

# **Arguments**

model	Any subset of "UUU" "CUU" "UCU" "CCU" "UCC" "UUC" "CUC", "CCC" indicating the fitted models.
nChains	The number of parallel heated chains. When 'dirPriorAlphas' is supplied, 'nChains' can be ignored.
dirPriorAlphas	vector of length nChains in the form of an increasing sequence of positive scalars. Each entry contains the (common) prior Dirichlet parameter for the corresponding chain. Default: dirPriorAlphas = $c(1, 1 + dN*(2:nChains - 1))/Kmax$ where dN = 1, for nChains > 1. Otherwise, dirPriorAlphas = $1/Kmax$ .
rawData	The observed data as an $n \times p$ matrix. Clustering is performed on the rows of the matrix.
outDir	Name of the output folder. An error is thrown if this directory already exists.
Kmax	Number of components in the overfitted mixture. Default: 20.
mCycles	Number of MCMC cycles. Each cycle consists of nIterPerCycle MCMC iterations. At the end of each cycle a swap of the state of two randomly chosen adjacent chains is attempted.
burnCycles	Number of cycles that will be discarded as burn-in period.
g	Prior parameter $g$ . Default value: $g = 0.5$ .
h	Prior parameter $h$ . Default value: $h = 0.5$ .
alpha_sigma	Prior parameter $\alpha$ . Default value: $\alpha = 0.5$ .
beta_sigma	Prior parameter $\beta$ . Default value: $\beta = 0.5$ .
q	A vector containing the number of factors to be fitted.
normalize	Should the observed data be normalized? Default value: TRUE. (Recommended)
thinning	Optional integer denoting the thinning of the keeped MCMC cycles.
zStart	Optional starting value for the allocation vector.
nIterPerCycle	Number of iteration per MCMC cycle. Default value: 10.

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gibbs\_z Select the gibbs sampling scheme for updating latent allocations of mixture model. Default value: 1.

warm\_up\_overfitting

Number of iterations for the overfitting initialization scheme. Default value: 500.

warm\_up Number of iterations that will be used to initialize the models before starting

proposing switchings. Default value: 5000.

overfittingInitialization

Logical value indicating whether the chains are initialized via the overfitting

initialization scheme. Default: TRUE.

progressGraphs Logical value indicating whether to plot successive states of the chains while the

sampler runs. Default: FALSE.

gwar Initialization parameter. Default: 0.05.

rmDir Logical value indicating whether to delete the outDir directory. Default: TRUE.

parallelModels Model-level parallelization: An optional integer specifying the number of cores

that will be used in order to fit in parallel each member of model.

### Value

An object of class fabMix.object (see the fabMix function).

#### Note

See the fabMix function for examples.

# Author(s)

Panagiotis Papastamoulis

fabMix\_UxC Function to estimate the UUC and UCC models

# **Description**

This function runs parallel chains under a prior tempering scheme of the Dirichlet prior distribution of mixture weights.

### Usage

```
fabMix_UxC(sameSigma, dirPriorAlphas, rawData, outDir, Kmax, mCycles,
burnCycles, g, h, alpha_sigma, beta_sigma, q, normalize,
thinning, zStart, nIterPerCycle, gibbs_z,
warm_up_overfitting, warm_up, overfittingInitialization,
progressGraphs, gwar)
```

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### **Arguments**

sameSigma Logical value denoting the parameterization of the error variance per compo-

nent. If TRUE, the parameterization CCU is fitted. Otherwise, the parameteriza-

tion CUU is fitted.

dirPriorAlphas The prior Dirichlet parameters for each chain.

rawData The observed data as an  $n \times p$  matrix. Clustering is performed on the rows of

the matrix.

outDir Name of the output folder.

Kmax Number of components in the overfitted mixture. Default: 20.

mCycles Number of MCMC cycles. Each cycle consists of nIterPerCycle MCMC it-

erations. At the end of each cycle a swap of the state of two randomly chosen

adjacent chains is attempted.

burnCycles Number of cycles that will be discarded as burn-in period.

g Prior parameter g. Default value: g=2. h Prior parameter h. Default value: h=1. alpha\_sigma Prior parameter  $\alpha$ . Default value:  $\alpha=2$ .

beta\_sigma Prior parameter  $\beta$ . Default value:  $\beta = 1$ .

Number of factors q, where  $1 \le q \le L$ . An error is thrown if the Ledermann

bound (L) is exceeded.

normalize Should the observed data be normalized? Default value: TRUE.

thinning Optional integer denoting the thinning of the keeped MCMC cycles.

zStart Optional starting value for the allocation vector.

nIterPerCycle Number of iteration per MCMC cycle. Default value: 10.

gibbs\_z Select the gibbs sampling scheme for updating latent allocations of mixture

model. Default value: 1.

warm\_up\_overfitting

Number of iterations for the overfitting initialization scheme. Default value:

100.

warm\_up Number of iterations that will be used to initialize the models before starting

proposing switchings. Default value: 500.

overfittingInitialization

Logical value indicating whether the chains are initialized via the overfitting

initialization scheme. Default: TRUE.

progressGraphs Logical value indicating whether to plot successive states of the chains while the

sampler runs. Default: FALSE.

gwar Initialization parameter. Default: 0.05.

### Value

List of files written to outDir

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### Note

It is recommended to always use: normalize = TRUE (default). Tuning of dirPriorAlphas may be necessary to achieve reasonable acceptance rates of chain swaps. Also note that the output is not identifiable due to label switching and the user has to subsequently call the dealWithLabelSwitching function. See the fabMix function for examples.

### Author(s)

Panagiotis Papastamoulis

### See Also

fabMix

fabMix\_UxU

Function to estimate the UUU and UCU model

### **Description**

This function runs parallel chains under a prior tempering scheme of the Dirichlet prior distribution of mixture weights.

# Usage

```
fabMix_UxU(sameSigma, dirPriorAlphas, rawData, outDir, Kmax, mCycles,
burnCycles, g, h, alpha_sigma, beta_sigma, q, normalize,
thinning, zStart, nIterPerCycle, gibbs_z,
warm_up_overfitting, warm_up, overfittingInitialization,
progressGraphs, gwar)
```

# **Arguments**

sameSigma	Logical value	denoting the	parameterization o	f the	error variance	per compo-
			parameter c			per compo

nent. If TRUE, the parameterization  $\Sigma_1 = \ldots = \Sigma_K$  is fitted.

dirPriorAlphas The prior Dirichlet parameters for each chain.

rawData The observed data as an  $n \times p$  matrix. Clustering is performed on the rows of

the matrix.

outDir Name of the output folder.

Kmax Number of components in the overfitted mixture. Default: 20.

mCycles Number of MCMC cycles. Each cycle consists of nIterPerCycle MCMC it-

erations. At the end of each cycle a swap of the state of two randomly chosen

adjacent chains is attempted.

burnCycles Number of cycles that will be discarded as burn-in period.

g Prior parameter g. Default value: g=2. h Prior parameter h. Default value: h=1.

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alpha\_sigma Prior parameter  $\alpha$ . Default value:  $\alpha=2$ . beta\_sigma Prior parameter  $\beta$ . Default value:  $\beta=1$ .

q Number of factors q, where  $1 \le q \le L$ . An error is thrown if the Ledermann

bound (L) is exceeded.

normalize Should the observed data be normalized? Default value: TRUE.

thinning Optional integer denoting the thinning of the keeped MCMC cycles.

zStart Optional starting value for the allocation vector.

nIterPerCycle Number of iteration per MCMC cycle. Default value: 10.

gibbs\_z Select the gibbs sampling scheme for updating latent allocations of mixture

model. Default value: 1.

warm\_up\_overfitting

Number of iterations for the overfitting initialization scheme. Default value:

100.

warm\_up Number of iterations that will be used to initialize the models before starting

proposing switchings. Default value: 500.

overfittingInitialization

Logical value indicating whether the chains are initialized via the overfitting

initialization scheme. Default: TRUE.

progressGraphs Logical value indicating whether to plot successive states of the chains while the

sampler runs. Default: FALSE.

gwar Initialization parameter. Default: 0.05.

#### Value

List of files written to outDir

## Note

It is recommended to always use: normalize = TRUE (default). Tuning of dirPriorAlphas may be necessary to achieve reasonable acceptance rates of chain swaps. Also note that the output is not identifiable due to label switching and the user has to subsequently call the dealWithLabelSwitching function. See the fabMix function for examples.

#### Author(s)

Panagiotis Papastamoulis

#### See Also

fabMix

38 getStuffForDIC

|--|

# Description

This function computes four information criteria for a given run of the fabMix algorithm, namely: AIC, BIC, DIC and DIC<sub>2</sub>. Given various runs with different number of factors, the selected model corresponds to the one with the smalled value of the selected criterion.

## Usage

 $getStuffForDIC(sameSigma, sameLambda, isotropic, x_data, outputFolder, q, burn, Km, normalize, discardLower)$ 

# Arguments

sameSigma	Logical value indicating whether the parameterization with the same variance of errors per component is used. Default: TRUE.
sameLambda	Logical value indicating whether the parameterization with same loadings per component is used. Default: FALSE.
isotropic	Logical value indicating whether the parameterization with isotropic error variance per component is used. Default: FALSE.
x_data	Observed data.
outputFolder	Name of the folder where the fabMix function has saved its output.
q	Number of factors. Note that this should coincide with the number of factors in the fabMix run.
burn	Discard observations as burn-in period (optional).
Km	Number of components in the overfitted mixture model. Note that this should coincide with the same entry in the fabMix run.
normalize	Should the observed data be normalized? Note that this should coincide with the same entry in the fabMix run. Default value: TRUE.
discardLower	Discard draws with log-likelihood values lower than the specific quantile. This applied only for the DIC computation.

## **Details**

If necessary, more details than the description above

# Value

The information criteria are saved to the informationCriteria\_map\_model.txt file in the code-outputFolder.

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## Note

It is well known that DIC tends to overfit, so it advised to compare models with different number of factors using AIC or BIC. The main function of the package uses BIC.

## Author(s)

Panagiotis Papastamoulis

 $log\_dirichlet\_pdf$ 

Log-density function of the Dirichlet distribution

# **Description**

Log-density function of the Dirichlet distribution

## Usage

```
log_dirichlet_pdf(alpha, weights)
```

# Arguments

alpha Parameter vector weights Vector of weights

# Value

Log-density of the  $D(alpha_1, \ldots, \alpha_k)$  evaluated at  $w_1, \ldots, w_k$ .

# Author(s)

Panagiotis Papastamoulis

myDirichlet

Simulate from the Dirichlet distribution

# **Description**

Generate a random draw from the Dirichlet distribution  $D(\alpha_1, \ldots, \alpha_k)$ .

# Usage

```
myDirichlet(alpha)
```

# **Arguments**

alpha

Parameter vector

### Value

Simulated vector

#### Author(s)

Panagiotis Papastamoulis

```
observed.log.likelihood0
```

Log-likelihood of the mixture model

# Description

Log-likelihood of the mixture model evaluated only at the alive components.

# Usage

```
observed.log.likelihood0(x_data, w, mu, Lambda, Sigma, z)
```

# **Arguments**

x\_data The observed data

w Vector of mixture weightsmu Vector of marginal means

Lambda Factor loadings

Sigma Diagonal of the common covariance matrix of the errors per cluster

z Allocation vector

## Value

Log-likelihood value

### Author(s)

Panagiotis Papastamoulis

```
library('fabMix')
data(waveDataset1500)
x_data <- waveDataset1500[ 1:20, -1] # data
z <- waveDataset1500[ 1:20, 1] # class
p <- dim(x_data)[2]
q <- 2
K <- length(table(z)) # 3 classes
# give some arbitrary values to the parameters:
set.seed(1)</pre>
```

```
w <- rep(1/K, K)
mu <- array( runif(K * p), dim = c(K,p) )
Lambda <- array( runif(K*p*q), dim = c(K,p,q) )
SigmaINV <- array(1, dim = c(p,p))
Sigma <- 1/diag(SigmaINV)
# compute the complete.log.likelihood
observed.log.likelihood0(x_data = x_data, w = w,
mu = mu, Lambda = Lambda, Sigma = Sigma, z = z)</pre>
```

```
observed.log.likelihood0_q0_sameSigma
```

Log-likelihood of the mixture model for q=0 and same variance of errors

#### **Description**

Log-likelihood of the mixture model evaluated only at the alive components.

## Usage

```
observed.log.likelihood0_q0_sameSigma(x_data, w, mu, Sigma, z)
```

## **Arguments**

x_data	The observed data
W	Vector of mixture weights
mu	Vector of marginal means
Sigma	Covariance matrix of the errors per cluster
Z	Allocation vector

## Value

Log-likelihood value

## Author(s)

Panagiotis Papastamoulis

```
library('fabMix')
data(waveDataset1500)
x_data <- waveDataset1500[ 1:20, -1] # data
z <- waveDataset1500[ 1:20, 1] # class
p <- dim(x_data)[2]
q <- 2
K <- length(table(z)) # 3 classes
# give some arbitrary values to the parameters:</pre>
```

```
set.seed(1)
w <- rep(1/K, K)
mu <- array( runif(K * p), dim = c(K,p) )
SigmaINV <- array(1, dim = c(p,p))
Sigma <- 1/diag(SigmaINV)
# compute the complete.log.likelihood
observed.log.likelihood0_q0_sameSigma(x_data = x_data, w = w,
mu = mu, Sigma = Sigma, z = z)</pre>
```

```
observed.log.likelihood0_Sj
```

Log-likelihood of the mixture model

## **Description**

Log-likelihood of the mixture model evaluated only at the alive components.

## Usage

```
observed.log.likelihood0_Sj(x_data, w, mu, Lambda, Sigma, z)
```

# **Arguments**

x_data	The observed data
W	Vector of mixture weights
mu	Vector of marginal means
Lambda	Factor loadings
Sigma	$K\times p$ matrix with each row containing the diagonal of the covariance matrix of the errors per cluster
Z	Allocation vector

# Value

Log-likelihood value

# Author(s)

Panagiotis Papastamoulis

```
library('fabMix')
data(waveDataset1500)
x_data <- waveDataset1500[ 1:20, -1] # data
z <- waveDataset1500[ 1:20, 1] # class
p <- dim(x_data)[2]
q <- 2</pre>
```

```
K <- length(table(z)) # 3 classes
# give some arbitrary values to the parameters:
set.seed(1)
w <- rep(1/K, K)
mu <- array( runif(K * p), dim = c(K,p) )
Lambda <- array( runif(K*p*q), dim = c(K,p,q) )
Sigma <- matrix(1:K, nrow = K, ncol = p)
# compute the complete.log.likelihood
observed.log.likelihood0_Sj(x_data = x_data, w = w, mu = mu, Lambda = Lambda, Sigma = Sigma, z = z)</pre>
```

```
observed.log.likelihood0_Sj_q0
```

Log-likelihood of the mixture model for q = 0

## **Description**

Log-likelihood of the mixture model evaluated only at the alive components.

## Usage

```
observed.log.likelihood0_Sj_q0(x_data, w, mu, Sigma, z)
```

### **Arguments**

x_data	The observed data
W	Vector of mixture weights
mu	Vector of marginal means
Sigma	$K \times p$ matrix with each row containing the diagonal of the covariance matrix of the errors per cluster
z	Allocation vector

### Value

Log-likelihood value

## Author(s)

Panagiotis Papastamoulis

```
library('fabMix')
data(waveDataset1500)
x_data <- waveDataset1500[ 1:20, -1] # data
z <- waveDataset1500[ 1:20, 1] # class
p <- dim(x_data)[2]
q <- 2</pre>
```

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```
K <- length(table(z)) # 3 classes
# give some arbitrary values to the parameters:
set.seed(1)
w <- rep(1/K, K)
mu <- array( runif(K * p), dim = c(K,p) )
Sigma <- matrix(1:K, nrow = K, ncol = p)
# compute the complete.log.likelihood
observed.log.likelihood0_Sj_q0(x_data = x_data, w = w,
mu = mu, Sigma = Sigma, z = z)</pre>
```

overfittingMFA

Basic MCMC sampler for the UCU model

## **Description**

Gibbs sampling for fitting a mixture model of factor analyzers.

# Usage

```
overfittingMFA(x_data, originalX, outputDirectory, Kmax, m, thinning, burn, g, h, alpha_prior, alpha_sigma, beta_sigma, start_values, q, zStart, gibbs_z)
```

### **Arguments**

x\_data normalized data

originalX observed raw data (only for plotting purpose)

outputDirectory

Name of the output folder

Kmax Number of mixture components

m Number of iterationsthinning Thinning of chainburn Burn-in period

g Prior parameter g. Default value: g=2. h Prior parameter h. Default value: h=1.

alpha\_prior Parameters of the Dirichlet prior distribution of mixture weights.

alpha\_sigma Prior parameter  $\alpha$ . Default value:  $\alpha=2$ . beta\_sigma Prior parameter  $\beta$ . Default value:  $\beta=1$ .

start\_values Optional (not used)
q Number of factors.
zStart Optional (not used)

gibbs\_z Optional

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### Value

Set of files written in outputDirectory.

### Author(s)

Panagiotis Papastamoulis

## **Examples**

```
library('fabMix')
n = 8
                     # sample size
p = 5
                     # number of variables
q = 2
                     # number of factors
K = 2
                    # true number of clusters
                         # diagonal of inverse variance of errors
sINV_diag = 1/((1:p))
set.seed(100)
syntheticDataset <- simData(sameLambda=TRUE, K.true = K, n = n, q = q, p = p,
                        sINV_values = sINV_diag)
colnames(syntheticDataset$data) <- paste0("x_",1:p)
Kmax <- 4
               # number of components for the overfitted mixture model
set.seed(1)
overfittingMFA(x_data = syntheticDataset$data,
originalX = syntheticDataset$data, outputDirectory = 'outDir',
Kmax = Kmax, m = 5, burn = 1,
g = 0.5, h = 0.5, alpha_prior = rep(1, Kmax),
alpha_sigma = 0.5, beta_sigma = 0.5,
start_values = FALSE, q = 2, gibbs_z = 1)
list.files('outDir')
unlink('outDir', recursive = TRUE)
```

overfittingMFA\_CCC

Basic MCMC sampler for the CCC model

## **Description**

Gibbs sampling for fitting a CCC mixture model of factor analyzers.

```
overfittingMFA_CCC(x_data, originalX, outputDirectory, Kmax, m, thinning, burn,
g, h, alpha_prior, alpha_sigma, beta_sigma,
start_values, q, zStart, gibbs_z)
```

## **Arguments**

x\_data normalized data

originalX observed raw data (only for plotting purpose)

outputDirectory

Name of the output folder

Kmax Number of mixture components

m Number of iterationsthinning Thinning of chainburn Burn-in period

g Prior parameter g. Default value: g=2. h Prior parameter h. Default value: h=1.

alpha\_prior Parameters of the Dirichlet prior distribution of mixture weights.

alpha\_sigma Prior parameter  $\alpha$ . Default value:  $\alpha=2$ . beta\_sigma Prior parameter  $\beta$ . Default value:  $\beta=1$ .

start\_values Optional (not used)
q Number of factors.
zStart Optional (not used)

gibbs\_z Optional

#### Value

Set of files written in outputDirectory.

#### Author(s)

Panagiotis Papastamoulis

```
library('fabMix')
n = 8
                     # sample size
                     # number of variables
p = 5
q = 2
                     # number of factors
K = 2
                     # true number of clusters
sINV_diag = 1/((1:p))
                         # diagonal of inverse variance of errors
set.seed(100)
syntheticDataset <- simData(sameLambda=TRUE, K.true = K, n = n, q = q, p = p,
                        sINV_values = sINV_diag)
colnames(syntheticDataset$data) <- paste0("x_",1:p)</pre>
Kmax <- 4
              # number of components for the overfitted mixture model
set.seed(1)
overfittingMFA_CCC <- overfittingMFA_CCC(x_data = syntheticDataset$data,</pre>
originalX = syntheticDataset$data, outputDirectory = 'outDir',
```

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```
Kmax = Kmax, m = 5, burn = 1,
g = 0.5, h = 0.5, alpha_prior = rep(1, Kmax),
alpha_sigma = 0.5, beta_sigma = 0.5,
start_values = FALSE, q = 2, gibbs_z = 1)
list.files('outDir')
unlink('outDir', recursive = TRUE)
```

overfittingMFA\_CCU

Basic MCMC sampler for the CCU model

# **Description**

Gibbs sampling for fitting a CCU mixture model of factor analyzers.

# Usage

```
overfittingMFA_CCU(x_data, originalX, outputDirectory, Kmax, m, thinning, burn, g, h, alpha_prior, alpha_sigma, beta_sigma, start_values, q, zStart, gibbs_z)
```

## **Arguments**

x\_data normalized data
originalX observed raw data (only for plotting purpose)

outputDirectory

Name of the output folder

Kmax Number of mixture components

m Number of iterationsthinning Thinning of chainburn Burn-in period

g Prior parameter g. Default value: g=2. h Prior parameter h. Default value: h=1.

alpha\_prior Parameters of the Dirichlet prior distribution of mixture weights.

alpha\_sigma Prior parameter  $\alpha$ . Default value:  $\alpha=2$ . beta\_sigma Prior parameter  $\beta$ . Default value:  $\beta=1$ .

q Optional (not used)
q Number of factors.
zStart Optional (not used)

gibbs\_z Optional

# Value

Set of files written in outputDirectory.

#### Author(s)

Panagiotis Papastamoulis

## **Examples**

```
library('fabMix')
n = 8
                     # sample size
p = 5
                     # number of variables
q = 2
                     # number of factors
K = 2
                     # true number of clusters
sINV_diag = 1/((1:p))
                         # diagonal of inverse variance of errors
set.seed(100)
syntheticDataset <- simData(sameLambda=TRUE,K.true = K, n = n, q = q, p = p,
                        sINV_values = sINV_diag)
colnames(syntheticDataset$data) <- paste0("x_",1:p)
Kmax <- 4
               # number of components for the overfitted mixture model
set.seed(1)
overfittingMFA_CCU(x_data = syntheticDataset$data,
originalX = syntheticDataset$data, outputDirectory = 'outDir',
Kmax = Kmax, m = 5, burn = 1,
g = 0.5, h = 0.5, alpha_prior = rep(1, Kmax),
alpha_sigma = 0.5, beta_sigma = 0.5,
start_values = FALSE, q = 2, gibbs_z = 1)
list.files('outDir')
unlink('outDir', recursive = TRUE)
```

overfittingMFA\_CUC

Basic MCMC sampler for the CUC model

# **Description**

Gibbs sampling for fitting a CUC mixture model of factor analyzers.

#### Usage

```
overfittingMFA_CUC(x_data, originalX, outputDirectory, Kmax, m, thinning, burn,
g, h, alpha_prior, alpha_sigma, beta_sigma,
start_values, q, zStart, gibbs_z)
```

## **Arguments**

```
x\_data normalized data originalX observed raw data (only for plotting purpose) outputDirectory Name of the output folder
```

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Number of mixture components Kmax Number of iterations thinning Thinning of chain Burn-in period burn Prior parameter g. Default value: g = 2. g Prior parameter h. Default value: h = 1. h alpha\_prior Parameters of the Dirichlet prior distribution of mixture weights. Prior parameter  $\alpha$ . Default value:  $\alpha = 2$ . alpha\_sigma beta\_sigma Prior parameter  $\beta$ . Default value:  $\beta = 1$ . start\_values Optional (not used) Number of factors. zStart Optional (not used) Optional gibbs\_z

#### Value

Set of files written in outputDirectory.

### Author(s)

Panagiotis Papastamoulis

```
library('fabMix')
n = 8
                     # sample size
p = 5
                     # number of variables
                     # number of factors
q = 2
K = 2
                     # true number of clusters
sINV_diag = 1/((1:p))
                         # diagonal of inverse variance of errors
set.seed(100)
syntheticDataset <- simData(sameLambda=TRUE,K.true = K, n = n, q = q, p = p,
                        sINV_values = sINV_diag)
colnames(syntheticDataset$data) <- paste0("x_",1:p)</pre>
Kmax <- 4
              # number of components for the overfitted mixture model
set.seed(1)
overfittingMFA_CUC(x_data = syntheticDataset$data,
originalX = syntheticDataset$data, outputDirectory = 'outDir',
Kmax = Kmax, m = 5, burn = 1,
g = 0.5, h = 0.5, alpha_prior = rep(1, Kmax),
alpha_sigma = 0.5, beta_sigma = 0.5,
start_values = FALSE, q = 2, gibbs_z = 1)
list.files('outDir')
unlink('outDir', recursive = TRUE)
```

overfittingMFA\_CUU

Basic MCMC sampler for the CUU model

## Description

Gibbs sampling for fitting a CUU mixture model of factor analyzers.

## Usage

```
overfittingMFA_CUU(x_data, originalX, outputDirectory, Kmax, m, thinning, burn, g, h, alpha_prior, alpha_sigma, beta_sigma, start_values, q, zStart, gibbs_z)
```

# **Arguments**

x\_data normalized data

originalX observed raw data (only for plotting purpose)

outputDirectory

Name of the output folder

Kmax Number of mixture components

m Number of iterationsthinning Thinning of chainburn Burn-in period

g Prior parameter g. Default value: g=2. h Prior parameter h. Default value: h=1.

alpha\_prior Parameters of the Dirichlet prior distribution of mixture weights.

alpha\_sigma Prior parameter  $\alpha$ . Default value:  $\alpha=2$ . beta\_sigma Prior parameter  $\beta$ . Default value:  $\beta=1$ .

start\_values Optional (not used)
q Number of factors.
zStart Optional (not used)

gibbs\_z Optional

## Value

Set of files written in outputDirectory.

## Author(s)

### **Examples**

```
library('fabMix')
n = 8
                     # sample size
p = 5
                     # number of variables
q = 2
                     # number of factors
K = 2
                     # true number of clusters
                         # diagonal of inverse variance of errors
sINV_diag = 1/((1:p))
set.seed(100)
syntheticDataset <- simData(sameLambda=TRUE, K.true = K, n = n, q = q, p = p,
                        sINV_values = sINV_diag)
colnames(syntheticDataset$data) <- paste0("x_",1:p)</pre>
Kmax <- 4
               # number of components for the overfitted mixture model
set.seed(1)
overfittingMFA_CUU(x_data = syntheticDataset$data,
originalX = syntheticDataset$data, outputDirectory = 'outDir',
Kmax = Kmax, m = 5, burn = 1,
g = 0.5, h = 0.5, alpha_prior = rep(1, Kmax),
alpha_sigma = 0.5, beta_sigma = 0.5,
start_values = FALSE, q = 2, gibbs_z = 1)
list.files('outDir')
unlink('outDir', recursive = TRUE)
```

overfittingMFA\_missing\_values

Basic MCMC sampler for the case of missing data

## **Description**

Gibbs sampling for fitting a mixture model of factor analyzers.

# Usage

```
overfittingMFA_missing_values(missing_entries, x_data, originalX, outputDirectory, Kmax,
m, thinning, burn, g, h, alpha_prior, alpha_sigma,
beta_sigma, start_values, q, zStart, gibbs_z)
```

## **Arguments**

```
missing_entries
```

list which contains the row number (1st entry) and column indexes (subsequent entries) for every row containing missing values.

x\_data normalized data

originalX observed raw data (only for plotting purpose)

outputDirectory

Name of the output folder

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Kmax Number of mixture components

m Number of iterationsthinning Thinning of chainburn Burn-in period

g Prior parameter g. Default value: g=2. h Prior parameter h. Default value: h=1.

alpha\_prior Parameters of the Dirichlet prior distribution of mixture weights.

alpha\_sigma Prior parameter  $\alpha$ . Default value:  $\alpha=2$ . beta\_sigma Prior parameter  $\beta$ . Default value:  $\beta=1$ .

q Optional (not used)
q Number of factors.
zStart Optional (not used)

gibbs\_z Optional

#### Value

List of files

### Author(s)

Panagiotis Papastamoulis

overfittingMFA\_Sj

Basic MCMC sampler for the UUU model

## **Description**

Gibbs sampling for fitting a mixture model of factor analyzers.

# Usage

```
overfittingMFA_Sj(x_data, originalX, outputDirectory, Kmax, m, thinning, burn, g, h, alpha_prior, alpha_sigma, beta_sigma, start_values, q, zStart, gibbs_z)
```

### **Arguments**

x\_data normalized data

originalX observed raw data (only for plotting purpose)

outputDirectory

Name of the output folder

Kmax Number of mixture components

m Number of iterations

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thinning	Thinning of chain
burn	Burn-in period
g	Prior parameter $g$ . Default value: $g = 2$ .
h	Prior parameter $h$ . Default value: $h = 1$ .
alpha_prior	Parameters of the Dirichlet prior distribution of mixture weights.
alpha_sigma	Prior parameter $\alpha$ . Default value: $\alpha = 2$ .
beta_sigma	Prior parameter $\beta$ . Default value: $\beta = 1$ .
start_values	Optional (not used)
q	Number of factors.
zStart	Optional (not used)
gibbs_z	Optional

#### Value

Set of files written in outputDirectory.

### Author(s)

Panagiotis Papastamoulis

```
library('fabMix')
n = 8
                    # sample size
p = 5
                    # number of variables
q = 2
                    # number of factors
K = 2
                    # true number of clusters
sINV_diag = 1/((1:p)) # diagonal of inverse variance of errors
set.seed(100)
syntheticDataset <- simData(sameLambda=TRUE,K.true = K, n = n, q = q, p = p,
                       sINV_values = sINV_diag)
colnames(syntheticDataset$data) <- paste0("x_",1:p)
            # number of components for the overfitted mixture model
Kmax <- 4
set.seed(1)
overfittingMFA_Sj(x_data = syntheticDataset$data,
originalX = syntheticDataset$data, outputDirectory = 'outDir',
Kmax = Kmax, m = 5, burn = 1,
g = 0.5, h = 0.5, alpha_prior = rep(1, Kmax),
alpha_sigma = 0.5, beta_sigma = 0.5,
start_values = FALSE, q = 2, gibbs_z = 1)
list.files('outDir')
unlink('outDir', recursive = TRUE)
```

```
overfittingMFA_Sj_missing_values
```

Basic MCMC sampler for the case of missing data and different error variance

## **Description**

Gibbs sampling for fitting a mixture model of factor analyzers.

## Usage

```
overfittingMFA_Sj_missing_values(missing_entries, x_data, originalX,
outputDirectory, Kmax,
m, thinning, burn, g, h, alpha_prior, alpha_sigma,
beta_sigma, start_values, q, zStart, gibbs_z)
```

## **Arguments**

missing\_entries

list which contains the row number (1st entry) and column indexes (subsequent

entries) for every row containing missing values.

x\_data normalized data

originalX observed raw data (only for plotting purpose)

outputDirectory

Name of the output folder

Kmax Number of mixture components

m Number of iterationsthinning Thinning of chainburn Burn-in period

g Prior parameter g. Default value: g=2. h Prior parameter h. Default value: h=1.

alpha\_prior Parameters of the Dirichlet prior distribution of mixture weights.

alpha\_sigma Prior parameter  $\alpha$ . Default value:  $\alpha=2$ . beta\_sigma Prior parameter  $\beta$ . Default value:  $\beta=1$ .

start\_values Optional (not used)
q Number of factors.
zStart Optional (not used)

gibbs\_z Optional

## Value

List of files

overfittingMFA\_UCC 55

### Author(s)

Panagiotis Papastamoulis

overfittingMFA\_UCC

Basic MCMC sampler for the UCC model

# Description

Gibbs sampling for fitting a UCC mixture model of factor analyzers.

### Usage

```
overfittingMFA_UCC(x_data, originalX, outputDirectory, Kmax, m, thinning, burn, g, h, alpha_prior, alpha_sigma, beta_sigma, start_values, q, zStart, gibbs_z)
```

## **Arguments**

x\_data normalized data

originalX observed raw data (only for plotting purpose)

outputDirectory

Name of the output folder

Kmax Number of mixture components

m Number of iterationsthinning Thinning of chainburn Burn-in period

g Prior parameter g. Default value: g=2. h Prior parameter h. Default value: h=1.

alpha\_prior Parameters of the Dirichlet prior distribution of mixture weights.

alpha\_sigma Prior parameter  $\alpha$ . Default value:  $\alpha=2$ . beta\_sigma Prior parameter  $\beta$ . Default value:  $\beta=1$ .

start\_values Optional (not used)
q Number of factors.
zStart Optional (not used)

gibbs\_z Optional

#### Value

Set of files written in outputDirectory.

## Author(s)

### **Examples**

```
library('fabMix')
n = 8
                     # sample size
p = 5
                     # number of variables
q = 2
                     # number of factors
K = 2
                     # true number of clusters
sINV_diag = 1/((1:p))
                         # diagonal of inverse variance of errors
set.seed(100)
syntheticDataset <- simData(sameLambda=TRUE, K.true = K, n = n, q = q, p = p,
                        sINV_values = sINV_diag)
colnames(syntheticDataset$data) <- paste0("x_",1:p)</pre>
Kmax <- 4
               # number of components for the overfitted mixture model
set.seed(1)
overfittingMFA_UCC(x_data = syntheticDataset$data,
originalX = syntheticDataset$data, outputDirectory = 'outDir',
Kmax = Kmax, m = 5, burn = 1,
g = 0.5, h = 0.5, alpha_prior = rep(1, Kmax),
alpha_sigma = 0.5, beta_sigma = 0.5,
start_values = FALSE, q = 2, gibbs_z = 1)
list.files('outDir')
unlink('outDir', recursive = TRUE)
```

overfittingMFA\_UUC

Basic MCMC sampler for the UUC model

## **Description**

Gibbs sampling for fitting a UUC mixture model of factor analyzers.

#### Usage

```
overfittingMFA_UUC(x_data, originalX, outputDirectory, Kmax, m, thinning, burn,
g, h, alpha_prior, alpha_sigma, beta_sigma,
start_values, q, zStart, gibbs_z)
```

# **Arguments**

thinning

x\_data normalized data observed raw data (only for plotting purpose) originalX outputDirectory Name of the output folder Number of mixture components Kmax Number of iterations Thinning of chain

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burn	Burn-in period
g	Prior parameter $g$ . Default value: $g = 2$ .
h	Prior parameter $h$ . Default value: $h = 1$ .
alpha_prior	Parameters of the Dirichlet prior distribution of mixture weights.
alpha_sigma	Prior parameter $\alpha$ . Default value: $\alpha = 2$ .
beta_sigma	Prior parameter $\beta$ . Default value: $\beta = 1$ .
start_values	Optional (not used)
q	Number of factors.
zStart	Optional (not used)
gibbs_z	Optional

## Value

Set of files written in outputDirectory.

#### Author(s)

Panagiotis Papastamoulis

```
library('fabMix')
n = 8
                                                                         # sample size
p = 5
                                                                        # number of variables
                                                                       # number of factors
q = 2
                                                                       # true number of clusters
K = 2
sINV\_diag = 1/((1:p)) # diagonal of inverse variance of errors
set.seed(100)
syntheticDataset <- simData(sameLambda=TRUE, K.true = K, n = n, q = q, p = p, q = q, p = q, p = q, p = p, q = q, p = q,
                                                                                    sINV_values = sINV_diag)
colnames(syntheticDataset$data) <- paste0("x_",1:p)
Kmax <- 4
                                      # number of components for the overfitted mixture model
set.seed(1)
overfittingMFA_UUC(x_data = syntheticDataset$data,
originalX = syntheticDataset$data, outputDirectory = 'outDir',
Kmax = Kmax, m = 5, burn = 1,
g = 0.5, h = 0.5, alpha_prior = rep(1, Kmax),
alpha_sigma = 0.5, beta_sigma = 0.5,
start_values = FALSE, q = 2, gibbs_z = 1)
list.files('outDir')
unlink('outDir', recursive = TRUE)
```

58 overfitting\_q0

overfitting_q0	MCMC sampler for $q=0$	

# Description

Gibbs sampling for fitting a mixture model with diagonal covariance structure.

## Usage

```
overfitting_q0(x_data, originalX, outputDirectory, Kmax, m, thinning, burn, g, h, alpha_prior, alpha_sigma, beta_sigma, start_values, q, zStart, gibbs_z)
```

# **Arguments**

x\_data normalized data

originalX observed raw data (only for plotting purpose)

outputDirectory

Name of the output folder

Kmax Number of mixture components

m Number of iterationsthinning Thinning of chainburnBurn-in period

g Prior parameter g. Default value: g=2. h Prior parameter h. Default value: h=1.

alpha\_prior Parameters of the Dirichlet prior distribution of mixture weights.

alpha\_sigma Prior parameter  $\alpha$ . Default value:  $\alpha=2$ . beta\_sigma Prior parameter  $\beta$ . Default value:  $\beta=1$ .

start\_values Optional (not used)
q Number of factors.
zStart Optional (not used)

gibbs\_z Optional

### Value

List of files

## Author(s)

```
overfitting_q0_sameSigma
```

MCMC sampler for q = 0 and same error variance parameterization

## **Description**

Gibbs sampling for fitting a mixture model with diagonal covariance structure.

## Usage

```
overfitting_q0_sameSigma(x_data, originalX, outputDirectory, Kmax, m, thinning, burn, g, h, alpha_prior, alpha_sigma, beta_sigma, start_values, q, zStart, gibbs_z)
```

# Arguments

x\_data normalized data

originalX observed raw data (only for plotting purpose)

outputDirectory

Name of the output folder

Kmax Number of mixture components

m Number of iterationsthinning Thinning of chainburn Burn-in period

g Prior parameter g. Default value: g=2. h Prior parameter h. Default value: h=1.

alpha\_prior Parameters of the Dirichlet prior distribution of mixture weights.

alpha\_sigma Prior parameter  $\alpha$ . Default value:  $\alpha=2$ . beta\_sigma Prior parameter  $\beta$ . Default value:  $\beta=1$ .

start\_values Optional (not used)
q Number of factors.
zStart Optional (not used)

gibbs\_z Optional

## Value

List of files

# Author(s)

60 plot.fabMix.object

plot.fabMix.object Plot function

#### **Description**

This function plots fabMix function.

# Usage

```
## S3 method for class 'fabMix.object'
plot(x, what, variableSubset, class_mfrow, sig_correlation,...)
```

### **Arguments**

x An object of class fabMix.object, which is returned by the fabMix function.

what One of the "BIC", "classification\_matplot", "classification\_pairs", "correlation",

"factor\_loadings". The plot will display the BIC values per model and number of factors (along with the most probable number of clusters as text), a matplot per cluster for the selected model, scatterplots pairs, the estimated correlation

matrix per cluster, and the MAP estimate of factor loadings, respectively.

variableSubset An optional subset of the variables. By default, all variables are selected.

class\_mfrow An optional integer vector of length 2, that will be used to set the mfrow for

"classification\_matplot" and "correlation" plots. By default, each plot is printed

to a new plotting area.

sig\_correlation

The "significance-level" for plotting the correlation between variables. Note that this is an estimate of a posterior probability and not a significance level as defined in frequentist statistics. Default value: NULL (all correlations are

plotted).

... ignored.

## Details

When the BIC values are plotted, a number indicates the most probable number of "alive" clusters. The pairwise scatterplots (what = "classification\_pairs") are created using the coordProj function of the mclust package. The what = "correlation" is plotted using the corrplot package. Note that the what = "classification\_matplot" plots the original data (before scaling and centering). On the other hand, the option what = "classification\_pairs" plots the centered and scaled data.

#### Author(s)

print.fabMix.object 61

### References

Luca Scrucca and Michael Fop and Thomas Brendan Murphy and Adrian E. Raftery (2017). mclust 5: clustering, classification and density estimation using Gaussian finite mixture models. The R Journal, 8(1): 205–233.

Taiyun Wei and Viliam Simko (2017). R package "corrplot": Visualization of a Correlation Matrix (Version 0.84). Available from https://github.com/taiyun/corrplot

# **Description**

This function prints a summary of objects returned by the fabMix function.

# Usage

```
## S3 method for class 'fabMix.object'
print(x, ...)
```

### **Arguments**

x An object of class fabMix.object, which is returned by the fabMix function.... ignored.

#### **Details**

The function prints some basic information for a fabMix.object.

## Author(s)

Panagiotis Papastamoulis

readLambdaValues Read Lambda values.

# Description

Function to read Lambda values from file.

```
readLambdaValues(myFile,K,p,q)
```

62 simData

# Arguments

myFile	File containing Lambda values
K	Number of components
p	Number of variables
q	Number of factors

## Value

 $K \times p \times q$  array of factor loadings.

# Author(s)

Panagiotis Papastamoulis

simData	Synthetic data generator

# Description

Simulate data from a multivariate normal mixture using a mixture of factor analyzers mechanism.

# Usage

```
simData(sameSigma, sameLambda, p, q, K.true, n, loading_means, loading_sd, sINV_values)
```

# Arguments

sameSigma	Logical.
sameLambda	Logical.
р	The dimension of the multivariate normal distribution $(p > 1)$ .
q	Number of factors. It should be strictly smaller than p.
K.true	The number of mixture components (clusters).
n	Sample size.
loading_means	A vector which contains the means of blocks of factor loadings.
	Default: loading_means = $c(-30, -20, -10, 10, 20, 30)$ .
loading_sd	A vector which contains the standard deviations of blocks of factor loadings.
	Default: loading_sd <- rep(2, length(loading_means)).
sINV_values	A vector which contains the values of the diagonal of the (common) inverse covariance matrix, if sigmaTrue = TRUE. An $K \times p$ matrix which contains the values of the diagonal of the inverse covariance matrix per component, if sigmaTrue = FALSE.
	Default: sINV_values = rgamma(p, shape = 1, rate = 1).

### Value

A list with the following entries:

data  $n \times p$  array containing the simulated data.

class *n*-dimensional vector containing the class of each observation.

factorLoadings  $K.true \times p \times q$ -array containing the factor loadings  $\Lambda_{krj}$  per cluster k, feature

r and factor j, where  $k = 1, \dots, K$ ;  $r = 1, \dots, p$ ;  $j = 1, \dots, q$ .

means  $K.true \times p$  matrix containing the marginal means  $\mu_{kr}$ , k = 1, ..., K; r =

 $1,\ldots,p$ .

variance  $p \times p$  diagonal matrix containing the variance of errors  $\sigma_{rr}$ ,  $r = 1, \dots, p$ . Note

that the same variance of errors is assumed for each cluster.

factors  $n \times q$  matrix containing the simulated factor values.

weights K.true-dimensional vector containing the weight of each cluster.

#### Note

The marginal variance for cluster k is equal to  $\Lambda_k \Lambda_k^T + \Sigma$ .

#### Author(s)

Panagiotis Papastamoulis

### **Examples**

summary.fabMix.object Summary method

## Description

S3 method for printing a summary of a fabMix.object.

```
## S3 method for class 'fabMix.object'
summary(object, quantile_probs, ...)
```

64 update\_all\_y

# Arguments

```
object An object of class fabMix.object, which is returned by the fabMix function.

quantile_probs A vector of quantiles to evaluate for each variable.

... Ignored.
```

#### **Details**

The function prints and returns a summary of the estimated posterior means for the parameters of the selected model for a fabMix.object. In particular, the method prints the ergodic means of the mixing proportions, marginal means and covariance matrix per component, as well as the corresponding quantiles.

#### Value

A list consisting of the following entries:

```
alive_cluster_labels
```

The labels of the "alive" components of the overfitting mixture model.

posterior\_means

Posterior means of mixing proportion, marginal means and covariance matrix

per (alive) cluster.

quantiles A matrix containing the quantiles for each parameter.

## Note

The summary function of the coda package to the mcmc object object\$mcmc is used for computing quantiles.

### Author(s)

Panagiotis Papastamoulis

update\_all\_y

Gibbs sampling for y in xCx model

#### **Description**

Gibbs sampling for updating the factors y for models with same variance of errors per component.

```
update_all_y(x_data, mu, SigmaINV, Lambda, z)
```

update\_all\_y\_Sj 65

## **Arguments**

```
x_data n \times p matrix with obseved data mu n \times p matrix of marginal means SigmaINV p \times p precision matrix Lambda p \times q matrix of factor loadings z Allocation vector
```

#### Value

A matrix with generated factors

## Author(s)

Panagiotis Papastamoulis

## **Examples**

```
library('fabMix')
n = 8
                     # sample size
                     # number of variables
p = 5
                    # number of factors
q = 2
K = 2
                     # true number of clusters
sINV_diag = 1/((1:p))
                         # diagonal of inverse variance of errors
set.seed(100)
syntheticDataset <- simData(sameLambda=TRUE, K.true = K, n = n, q = q, p = p, q)
                        sINV_values = sINV_diag)
# use the real values as input and simulate factors
update_all_y(x_data = syntheticDataset$data,
mu = syntheticDataset$means,
SigmaINV = diag(1/diag(syntheticDataset$variance)),
Lambda = syntheticDataset$factorLoadings,
z = syntheticDataset$class)
```

update\_all\_y\_Sj

Gibbs sampling for y in xUx model

## **Description**

Gibbs sampling for updating the factors y for models with different variance of errors per component.

```
update_all_y_Sj(x_data, mu, SigmaINV, Lambda, z)
```

66 update\_OmegaINV

# **Arguments**

x\_data  $n\times p \text{ matrix with obseved data}$  mu  $n\times p \text{ matrix of marginal means}$ 

SigmaINV  $K \times p \times p$  array containing the precision matrix per component

Lambda  $p \times q$  matrix of factor loadings

z Allocation vector

### Value

A matrix with generated factors

## Author(s)

Panagiotis Papastamoulis

# **Examples**

```
library('fabMix')
                     # sample size
n = 8
p = 5
                     # number of variables
q = 2
                    # number of factors
                    # true number of clusters
sINV_diag = 1/((1:p))
                         # diagonal of inverse variance of errors
set.seed(100)
syntheticDataset < simData(sameLambda=TRUE, K.true = K, n = n, q = q, p = p,
                        sINV_values = sINV_diag)
# add some noise here:
SigmaINV <- array(data = 0, dim = c(K,p,p))
for(k in 1:K){
     diag(SigmaINV[k,,]) < -1/diag(syntheticDataset$variance) + rgamma(p, shape=1, rate = 1)
# use the real values as input and simulate factors
update_all_y_Sj(x_data = syntheticDataset$data,
mu = syntheticDataset$means,
SigmaINV = SigmaINV,
Lambda = syntheticDataset$factorLoadings,
z = syntheticDataset$class)
```

update\_OmegaINV

Gibbs sampling for  $\Omega^-1$ 

# **Description**

Gibbs sampling for  $\Omega^{-1}$ 

### Usage

```
update_OmegaINV(Lambda, K, g, h)
```

### **Arguments**

Lambda	Factor loadings
K	Number of components
g	Prior parameter
h	Prior parameter

### Value

```
q \times q matrix \Omega^{-1}
```

## Author(s)

Panagiotis Papastamoulis

## **Examples**

```
library('fabMix')
# simulate some data
                     # sample size
p = 5
                     # number of variables
q = 2
                     # number of factors
K = 2
                     # true number of clusters
sINV_diag = 1/((1:p)) # diagonal of inverse variance of errors
set.seed(100)
syntheticDataset <- simData(sameLambda=TRUE,K.true = K, n = n, q = q, p = p,</pre>
                        sINV_values = sINV_diag)
SigmaINV <- array(data = 0, dim = c(K,p,p))
for(k in 1:K){
     diag(SigmaINV[k,,]) \leftarrow 1/diag(syntheticDataset$variance) + rgamma(p, shape=1, rate = 1)
}
# use the real values as input and simulate allocations
update_OmegaINV(Lambda = syntheticDataset$factorLoadings,
        K = K, g=0.5, h = 0.5
```

 $\label{eq:constraints} \mbox{update\_OmegaINV\_Cxx} \qquad \mbox{\it Gibbs sampling for $\Omega^-$-1 for $C\!xx$ model}$ 

# Description

Gibbs sampling for  $\Omega^{-1}$  for Cxx model

### Usage

```
update_OmegaINV_Cxx(Lambda, K, g, h)
```

# Arguments

Lambda	Factor loadings, in the form of $K \times p \times q$ matrix, under the restriction that all components share the factor loadings.
K	Number of components
g	Prior parameter
h	Prior parameter

#### Value

```
q \times q matrix \Omega^{-1}
```

### Author(s)

Panagiotis Papastamoulis

```
library('fabMix')
# simulate some data
n = 8
                     # sample size
p = 5
                     # number of variables
q = 2
                     # number of factors
K = 2
                     # true number of clusters
sINV\_diag = 1/((1:p)) # diagonal of inverse variance of errors
set.seed(100)
syntheticDataset <- simData(sameLambda=TRUE, K.true = K, n = n, q = q, p = p, q)
                        sINV_values = sINV_diag)
SigmaINV <- array(data = 0, dim = c(K,p,p))
for(k in 1:K){
     \label{eq:continuous} diag(SigmaINV[k,,]) <- 1/diag(syntheticDataset$variance) + rgamma(p, shape=1, rate = 1)
}
# Use the real values as input and simulate allocations.
# Mmake sure that in this case Lambda[k,,] is the same
# for all k = 1, \ldots, K
update_OmegaINV_Cxx(Lambda = syntheticDataset$factorLoadings,
        K = K, g=0.5, h = 0.5
```

```
update_SigmaINV_faster {\it Gibbs\ sampling\ for\ } \Sigma^{\hat{}} - 1
```

# **Description**

Gibbs sampling for updating  $\Sigma^{-1}$  for the xCU model.

## Usage

```
update_SigmaINV_faster(x_data, z, y, Lambda, mu, K, alpha_sigma, beta_sigma)
```

## **Arguments**

x_data	$n \times p$ matrix containing the observed data
z	Allocation vector
У	$n \times q$ matrix containing the latent factors
Lambda	$K \times p \times q$ array with factor loadings
mu	$K \times p$ array containing the marginal means
K	Number of components
alpha_sigma	Prior parameter alpha
beta_sigma	Prior parameter $beta$

## Value

 $p \times p$  matrix with the common variance of errors per component  $\Sigma^{-1}$ .

## Author(s)

Panagiotis Papastamoulis

```
library('fabMix')
# simulate some data
n = 8
                    # sample size
p = 5
                    # number of variables
                    # number of factors
q = 2
K = 2
                     # true number of clusters
sINV_diag = 1/((1:p))
                       # diagonal of inverse variance of errors
set.seed(100)
syntheticDataset <- simData(sameLambda=TRUE,K.true = K, n = n, q = q, p = p,
                        sINV_values = sINV_diag)
# use the real values as input and update SigmaINV
update_SigmaINV_faster(x_data = syntheticDataset$data,
```

```
z = syntheticDataset$class,
y = syntheticDataset$factors,
Lambda = syntheticDataset$factorLoadings,
mu = syntheticDataset$means,
K = K,
alpha_sigma = 0.5, beta_sigma = 0.5)
```

```
update_SigmaINV_faster_q0  {\it Gibbs\ sampling\ for\ } \Sigma^{\hat{}} - 1\ per\ component\ for\ q = 0
```

# Description

Gibbs sampling for  $\Sigma^{-1}$  per component

# Usage

```
update_SigmaINV_faster_q0( z, mu, K, alpha_sigma, beta_sigma, x_data)
```

# Arguments

z Allocation vector mu Marginal means

K Number of components

alpha\_sigma Prior parameter beta\_sigma Prior parameter

x\_data Data

# Value

 $\Sigma^{-1}$ 

# Author(s)

```
update_SigmaINV_faster_q0_sameSigma  
  {\it Gibbs\ sampling\ for\ } \Sigma^{\hat{}}-1\ per\ component\ for\ q=0
```

# **Description**

Gibbs sampling for  $\Sigma^{-1}$  per component

## Usage

```
update_SigmaINV_faster_q0_sameSigma( z, mu, K, alpha_sigma, beta_sigma, x_data)
```

## **Arguments**

Z	Allocation vector
mu	Marginal means

K Number of components

alpha\_sigma Prior parameter beta\_sigma Prior parameter

x\_data Data

## Value

 $\Sigma^{-1}$ 

# Author(s)

Panagiotis Papastamoulis

```
update_SigmaINV_faster_Sj {\it Gibbs\ sampling\ for\ } \Sigma^{\hat{}} - 1\ per\ component
```

# Description

Gibbs sampling for updating  $\Sigma^{-1}$  for the xUU model.

```
update_SigmaINV_faster_Sj(x_data, z, y, Lambda, mu, K, alpha_sigma, beta_sigma)
```

## **Arguments**

x_data	$n \times p$ matrix containing the observed data
z	Allocation vector
у	$n \times q$ matrix containing the latent factors
Lambda	$K\times p\times q$ array with factor loadings
mu	$K \times p$ array containing the marginal means
K	Number of components
alpha_sigma	Prior parameter $\alpha$
beta_sigma	Prior parameter $\beta$

## Value

 $K \times p \times p$  array with the variance of errors per component  $\Sigma_k^{-1}$ ,  $k=1,\ldots,K$ .

### Author(s)

Panagiotis Papastamoulis

```
library('fabMix')
# simulate some data
n = 8
                    # sample size
                    # number of variables
p = 5
q = 2
                    # number of factors
K = 2
                    # true number of clusters
                      # diagonal of inverse variance of errors
sINV_diag = 1/((1:p))
set.seed(100)
syntheticDataset <- simData(sameLambda=TRUE, K.true = K, n = n, q = q, p = p, q)
                       sINV_values = sINV_diag)
# use the real values as input and update SigmaINV
update_SigmaINV_faster_Sj(x_data = syntheticDataset$data,
z = syntheticDataset$class,
y = syntheticDataset$factors,
Lambda = syntheticDataset$factorLoadings,
mu = syntheticDataset$means,
K = K,
alpha_sigma = 0.5, beta_sigma = 0.5)
```

```
update_SigmaINV_xCC Gibbs sampling for \Sigma^-1 for xCC models
```

## **Description**

Gibbs sampling for  $\Sigma^{-1}$  for xCC models

## Usage

```
update_SigmaINV_xCC(x_data, z, y, Lambda, mu, K, alpha_sigma, beta_sigma)
```

## **Arguments**

x_data	$n \times p$ matrix containing the observed data
Z	Allocation vector
У	$n \times q$ matrix containing the latent factors
Lambda	$K \times p \times q$ array with factor loadings
mu	$K \times p$ array containing the marginal means
K	Number of components
alpha_sigma	Prior parameter $alpha$
beta_sigma	Prior parameter $beta$

#### Value

 $p \times p$  matrix with the common variance of errors per component  $\Sigma^{-1} = \sigma I_p$ .

## Author(s)

Panagiotis Papastamoulis

# **Examples**

```
library('fabMix')
# simulate some data
n = 8
                    # sample size
p = 5
                    # number of variables
q = 2
                    # number of factors
                    # true number of clusters
K = 2
sINV_diag = 1/((1:p))
                       # diagonal of inverse variance of errors
set.seed(100)
syntheticDataset <- simData(sameLambda=TRUE,K.true = K, n = n, q = q, p = p,
                       sINV_values = sINV_diag)
# use the real values as input and update SigmaINV
update_SigmaINV_xCC(x_data = syntheticDataset$data,
z = syntheticDataset$class,
y = syntheticDataset$factors,
```

```
Lambda = syntheticDataset$factorLoadings,
mu = syntheticDataset$means,
K = K,
alpha_sigma = 0.5, beta_sigma = 0.5)
```

update\_SigmaINV\_xUC

Gibbs sampling for  $\Sigma^-1$  per component for xUC models

## **Description**

Gibbs sampling for  $\Sigma^{-1}$  per component for xUC models

# Usage

```
update_SigmaINV_xUC(x_data, z, y, Lambda, mu, K, alpha_sigma, beta_sigma)
```

## **Arguments**

x\_data  $n \times p$  matrix containing the observed data

z Allocation vector

y  $n\times q \text{ matrix containing the latent factors}$  Lambda  $K\times p\times q \text{ array with factor loadings}$ 

mu  $K \times p$  array containing the marginal means

K Number of components alpha\_sigma Prior parameter alpha beta\_sigma Prior parameter beta

#### Value

 $K \times p \times p$  array containing the inverse variance of errors per component under the restriction:  $\Sigma_k^{-1} = \sigma_k I_p$ , where  $\sigma_k > 0$ .

## Author(s)

Panagiotis Papastamoulis

## **Examples**

update\_z2 75

update\_z2

Collapsed Gibbs for z using matrix inversion lemma

# Description

Collapsed Gibbs for z using matrix inversion lemma

## Usage

```
update_z2(w, mu, Lambda, SigmaINV, K, x_data)
```

## **Arguments**

w vector with length K consisting of mixture weights

mu  $K \times p$  array containing the marginal means

Lambda  $K \times p$  array with factor loadings

SigmaINV  $p \times p$  precision matrix K Number of components

x\_data  $n \times p$  matrix containing the observed data

#### Value

Allocation vector

## Author(s)

Panagiotis Papastamoulis

76 update\_z2\_Sj

## **Examples**

```
library('fabMix')
# simulate some data
n = 8
                    # sample size
p = 5
                    # number of variables
                    # number of factors
q = 2
                    # true number of clusters
K = 2
sINV_diag = 1/((1:p))
                       # diagonal of inverse variance of errors
set.seed(100)
syntheticDataset <- simData(sameLambda=TRUE,K.true = K, n = n, q = q, p = p,
                       sINV_values = sINV_diag)
# use the real values as input and simulate allocations
update_z2(w = syntheticDataset$weights, mu = syntheticDataset$means,
Lambda = syntheticDataset$factorLoadings,
SigmaINV = diag(1/diag(syntheticDataset$variance)),
K = K, x_data = syntheticDataset$data)$z
```

update\_z2\_Sj

Collapsed Gibbs for z using matrix inversion lemma

## Description

Collapsed Gibbs for z using matrix inversion lemma

## Usage

```
update_z2_Sj(w, mu, Lambda, SigmaINV, K, x_data)
```

#### **Arguments**

w vector with length K consisting of mixture weights

mu  $K \times p$  array containing the marginal means

Lambda  $K \times p$  array with factor loadings

SigmaINV  $K \times p \times p$  array containing the precision matrix per component

K Number of components

x\_data  $n \times p$  matrix containing the observed data

#### Value

Allocation vector

## Author(s)

Panagiotis Papastamoulis

update\_z4 77

## **Examples**

```
library('fabMix')
# simulate some data
                     # sample size
p = 5
                    # number of variables
q = 2
                    # number of factors
K = 2
                     # true number of clusters
sINV_diag = 1/((1:p))
                       # diagonal of inverse variance of errors
set.seed(100)
syntheticDataset <- simData(sameLambda=TRUE,K.true = K, n = n, q = q, p = p,
                        sINV_values = sINV_diag)
SigmaINV <- array(data = 0, dim = c(K,p,p))
for(k in 1:K){
diag(SigmaINV[k,,]) <- 1/diag(syntheticDataset$variance) + rgamma(p, shape=1, rate = 1)</pre>
# use the real values as input and simulate allocations
update_z2_Sj(w = syntheticDataset$weights, mu = syntheticDataset$means,
Lambda = syntheticDataset$factorLoadings,
SigmaINV = SigmaINV,
K = K, x_data = syntheticDataset$data)$z
```

update\_z4

Collapsed Gibbs for z

## **Description**

Collapsed Gibbs for z.

#### **Usage**

```
update_z4(w, mu, Lambda, SigmaINV, K, x_data)
```

#### **Arguments**

w vector with length K consisting of mixture weights mu  $K \times p$  array containing the marginal means Lambda  $K \times p$  array with factor loadings

SigmaINV  $p \times p$  precision matrix K Number of components

x\_data  $n \times p$  matrix containing the observed data

#### Value

A vector of length n with the simulated allocation of each observation among the K components.

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## Author(s)

Panagiotis Papastamoulis

## **Examples**

```
library('fabMix')
# simulate some data
n = 8
                     # sample size
p = 5
                    # number of variables
q = 2
                    # number of factors
                    # true number of clusters
K = 2
sINV_diag = 1/((1:p)) # diagonal of inverse variance of errors
set.seed(100)
syntheticDataset <- simData(sameLambda=TRUE,K.true = K, n = n, q = q, p = p,</pre>
                        sINV_values = sINV_diag)
# use the real values as input and simulate allocations
update_z4(w = syntheticDataset$weights, mu = syntheticDataset$means,
Lambda = syntheticDataset$factorLoadings,
SigmaINV = diag(1/diag(syntheticDataset$variance)),
K = K, x_data = syntheticDataset$data)$z
```

update\_z4\_Sj

Collapsed Gibbs for z

## **Description**

Collapsed Gibbs for z

#### **Usage**

```
update_z4_Sj(w, mu, Lambda, SigmaINV, K, x_data)
```

# **Arguments**

w vector with length K consisting of mixture weights

mu  $K \times p$  array containing the marginal means

Lambda  $K \times p$  array with factor loadings

SigmaINV  $K \times p \times p$  array containing the precision matrix per component

K Number of components

x\_data  $n \times p$  matrix containing the observed data

#### Value

Allocation vector

update\_z\_b

## Author(s)

Panagiotis Papastamoulis

## **Examples**

```
library('fabMix')
# simulate some data
n = 8
                     # sample size
p = 5
                     # number of variables
q = 2
                    # number of factors
                    # true number of clusters
K = 2
sINV_diag = 1/((1:p)) # diagonal of inverse variance of errors
set.seed(100)
syntheticDataset <- simData(sameLambda=TRUE, K.true = K, n = n, q = q, p = p,
                        sINV_values = sINV_diag)
SigmaINV <- array(data = 0, dim = c(K,p,p))
for(k in 1:K){
diag(SigmaINV[k,,]) <- 1/diag(syntheticDataset$variance) + rgamma(p, shape=1, rate = 1)</pre>
# use the real values as input and simulate allocations
update_z4_Sj(w = syntheticDataset$weights, mu = syntheticDataset$means,
Lambda = syntheticDataset$factorLoadings,
SigmaINV = SigmaINV,
K = K, x_{data} = syntheticDataset$data)$z
```

update\_z\_b

Gibbs sampling for z

## **Description**

Gibbs sampling for z: here the full conditional distribution is being used (that is, the distribution is also conditioned on the values of factors y).

## Usage

```
update_z_b(w, mu, Lambda, y, SigmaINV, K, x_data)
```

## **Arguments**

w vector with length K consisting of mixture weights mu  $K \times p$  array containing the marginal means  $K \times p$  array with factor loadings y  $n \times q$  Matrix of factors SigmaINV Precision matrix K Number of components  $\mathbf{x}_{-}$ data Data

80 update\_z\_b\_Sj

## Value

Allocation vector

## Author(s)

Panagiotis Papastamoulis

## **Examples**

```
library('fabMix')
# simulate some data
n = 8
                    # sample size
p = 5
                    # number of variables
q = 2
                    # number of factors
K = 2
                    # true number of clusters
sINV\_diag = 1/((1:p)) # diagonal of inverse variance of errors
set.seed(100)
syntheticDataset <- simData(sameLambda=TRUE, K.true = K, n = n, q = q, p = p, q)
                       sINV_values = sINV_diag)
# use the real values as input and simulate allocations
update_z_b(w = syntheticDataset$weights, mu = syntheticDataset$means,
Lambda = syntheticDataset$factorLoadings,
y = syntheticDataset$factors,
SigmaINV = diag(1/diag(syntheticDataset$variance)),
K = K, x_data = syntheticDataset$data)$z
```

update\_z\_b\_Sj

Gibbs sampling for z

## **Description**

Gibbs sampling for z: here the full conditional distribution is being used (that is, the distribution is also conditioned on the values of factors y).

## Usage

```
update_z_b_Sj(w, mu, Lambda, y, SigmaINV, K, x_data)
```

## **Arguments**

W	vector with length $K$ consisting of mixture weights
mu	$K \times p$ array containing the marginal means
Lambda	$K \times p$ array with factor loadings
у	$n \times q$ Matrix of factors
SigmaINV	$K \times p \times p$ array containing the precision matrix per component
K	Number of components
x_data	$n \times p$ matrix containing the observed data

 $update\_z\_q0$  81

## Value

Allocation vector

## Author(s)

Panagiotis Papastamoulis

# Examples

```
library('fabMix')
# simulate some data
n = 8
                    # sample size
p = 5
                    # number of variables
q = 2
                    # number of factors
K = 2
                    # true number of clusters
sINV_diag = 1/((1:p))
                      # diagonal of inverse variance of errors
set.seed(100)
syntheticDataset <- simData(sameLambda=TRUE,K.true = K, n = n, q = q, p = p,</pre>
                       sINV_values = sINV_diag)
SigmaINV <- array(data = 0, dim = c(K,p,p))
for(k in 1:K){
diag(SigmaINV[k,,]) <- 1/diag(syntheticDataset$variance) + rgamma(p, shape=1, rate = 1)
}
# use the real values as input and simulate allocations
update_z_b_Sj(w = syntheticDataset$weights, mu = syntheticDataset$means,
Lambda = syntheticDataset$factorLoadings,
v = syntheticDataset$factors,
SigmaINV = SigmaINV,
K = K, x_data = syntheticDataset$data)$z
```

update\_z\_q0

Gibbs sampling for z for q = 0

## **Description**

Gibbs sampling for z

## Usage

```
update_z_q0(w, mu, SigmaINV, K, x_data)
```

## **Arguments**

W	Mixture weights
mu	Marginal means

SigmaINV Precision matrix per component

K Number of components

x\_data Data

# Value

Allocation vector

# Author(s)

Panagiotis Papastamoulis

```
{\tt update\_z\_q0\_sameSigma} \quad \textit{Gibbs sampling for } z \textit{ for } q = 0
```

# Description

Gibbs sampling for z

# Usage

```
update_z_q0_sameSigma(w, mu, SigmaINV, K, x_data)
```

# Arguments

mu

w Mixture weights

SigmaINV Precision matrix per component

Marginal means

K Number of components

x\_data Data

# Value

Allocation vector

# Author(s)

Panagiotis Papastamoulis

waveDataset1500 83

waveDataset1500

Wave dataset

# Description

A subset of 1500 randomly sampled observations from the wave dataset (version 1), available from the UCI machine learning repository. It contains 3 classes of waves (variable class with values "1", "2" and "3") and 21 attributes. Each class is generated from a combination of 2 of 3 base waves with noise.

## Usage

waveDataset1500

## **Format**

A data frame with 1500 rows and 22 columns. The first column denotes the class of each observation.

#### Source

https://archive.ics.uci.edu/ml/datasets/Waveform+Database+Generator+(Version+1)

#### References

Lichman, M. (2013). UCI Machine Learning Repository http://archive.ics.uci.edu/ml. Irvine, CA: University of California, School of Information and Computer Science.

Breiman, L., Friedman, J.H., Olshen, R.A. and Stone, C.J. (1984). Classification and Regression Trees. Wadsworth International Group: Belmont, California.

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