# Package 'fabMix'

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Title Overfitting Parsimonious Bayesian Mixtures of Factor Analyzers

with an Unknown Number of Components

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Description Model-based clustering of multivariate continuous data using overfitting Bayesian mixtures of factor analyzers (Papastamoulis, 2018 CSDA). Suitable prior assumptions ensure that asymptotically the extra components will have zero posterior weight (empty), therefore, the inference on the number of clusters is based on the ``alive" components. The number of factors is considered fixed, and the optimal one can be estimated using information criteria. Eight parameterizations are available, namely the ``UUU", ``UCU", ``UCC", ``CUU", ``CUC", ``CCC", ``CCU" and ``UUC" models (see McNicholas et al, 2008 Stat Comp). Identifiability issues related to label switching are dealt by post-processing the simulated output with the ECR algorithm (Papastamoulis 2010 JCGS, 2016 JSS). Missing values are currently allowed for the UUU and UCU model parameterizations.
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fabMix-package3complete.log.likelihood4complete.log.likelihood_q05complete.log.likelihood_q0_sameSigma6complete.log.likelihood_Sj6compute_A_B_G_D_and_simulate_mu_Lambda7

compute_A_B_G_D_and_simulate_mu_Lambda_CCU	8
compute_A_B_G_D_and_simulate_mu_Lambda_CUU	9
compute_A_B_G_D_and_simulate_mu_Lambda_q0	9
compute_A_B_G_D_and_simulate_mu_Lambda_q0_sameSigma	10
compute_A_B_G_D_and_simulate_mu_Lambda_Sj	11
compute_sufficient_statistics	12
compute_sufficient_statistics_given_mu	12
compute_sufficient_statistics_q0	13
dealWithLabelSwitching	14
fabMix	15
fabMix_CxC	17
fabMix_CxU	20
fabMix_missing_values	22
fabMix_UxC	24
fabMix_UxU	27
getStuffForDIC	29
log_dirichlet_pdf	31
myDirichlet	31 32
$\epsilon$	32 32
6 -1 - 6	
observed.log.likelihood0_Sj	33
observed.log.likelihood0_Sj_q0	34
overfittingMFA	34
overfittingMFA_CCC	35
overfittingMFA_CCU	
overfittingMFA_CUC	
overfittingMFA_CUU	
overfittingMFA_missing_values	39
overfittingMFA_Sj	40
overfittingMFA_Sj_missing_values	41
overfittingMFA_UCC	42
overfittingMFA_UUC	43
overfitting_q0	44
overfitting_q0_sameSigma	45
plot.fabMix.object	46
print.fabMix.object	47
readLambdaValues	48
simData	48
update_all_y	50
update_all_y_Si	50
update OmegaINV	51
update OmegaINV Cxx	52
update_SigmaINV_faster	52
update_SigmaINV_faster_q0	53
update_SigmaINV_faster_q0_sameSigma	54
update_SigmaINV_faster_Sj	54
update_SigmaINV_xCC	55
update_SigmaINV_xUC	56
	- 0

fabMix-p	1	2
ton//liv n	nackada	4
IADIVITA-D	Dackage	.)

fabM:	ix-package	Overfit an Unk			-		xtı	ıres	of	Fα	icte	or.	An	aly	ze	rs	wit	h
Index																		63
	waveDataset1500		 	 	 	•						•	•		•	•		62
	update_z_q0_same	Sigma .	 	 	 													61
	update_z_q0		 	 	 													61
	update_z_b_Sj		 	 	 													60
	update_z_b		 	 	 													59
	update_z4_Sj		 	 	 													59
	update_z4		 	 	 													58
	update_z2_Sj		 	 	 													57
	update_z2		 	 	 													57

#### **Description**

Model-based clustering of multivariate continuous data using overfitting Bayesian mixtures of factor analyzers (Papastamoulis, 2018 CSDA). Suitable prior assumptions ensure that asymptotically the extra components will have zero posterior weight (empty), therefore, the inference on the number of clusters is based on the "alive" components. The number of factors is considered fixed, and the optimal one can be estimated using information criteria. Eight parameterizations are available, namely the "UUU", "UCU", "UCC", "CUU", "CUC", "CCC", "CCU" and "UUC" models (see McNicholas et al, 2008 Stat Comp). Identifiability issues related to label switching are dealt by post-processing the simulated output with the ECR algorithm (Papastamoulis 2010 JCGS, 2016 JSS). Missing values are currently allowed for the UUU and UCU model parameterizations.

#### Author(s)

Panagiotis Papastamoulis

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#### References

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

McNicholas, P.D. and Murphy, T.B. Stat Comput (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.

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**

```
library('fabMix')
n = 10
                     # sample size
p = 8
                     # number of variables
q = 2
                     # number of factors
K = 2
           # 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$data) <- paste0("x_",1:p)
qRange <- 1:2 # range of values for the number of factors
Kmax <- 5 # number of components for the overfitted mixture model
nChains <- 2 # number of parallel heated chains
                 # parameter the controls difference between successive chains
dirPriorAlphas <- c(1, 1 + dN * (2:nChains - 1))/Kmax # Dirichlet prior parameter per chain
set.seed(1)
fm <- fabMix( model = c("UCU", "UUC"), dirPriorAlphas = dirPriorAlphas,</pre>
rawData = syntheticDataset$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 = 5, warm_up = 25)
# 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 = 8, mCycles = 1100, burnCycles = 100,
         warm_up_overfitting = 500, warm_up = 10000.
print(fm)
plot(fm, what = "BIC")
plot(fm, what = "classification_pairs")
```

complete.log.likelihood

Complete log-likelihood function

#### **Description**

Complete log-likelihood function

### Usage

```
complete.log.likelihood(x\_data,\ w,\ mu,\ Lambda,\ SigmaINV,\ z)
```

#### **Arguments**

x\_data Data

w Mixture weightsmu Marginal meansLambda Factor loadings

SigmaINV Precision matrix (inverse covariance)

z Allocation vector of the data to the mixture components

#### Value

complete log-likelihood value

#### Author(s)

Panagiotis Papastamoulis

```
complete.log.likelihood_q0
```

Complete log-likelihood function for q = 0

### **Description**

Complete log-likelihood function

### Usage

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

### **Arguments**

x\_data Data

w Mixture weightsmu Marginal means

SigmaINV Precision matrix (inverse covariance)

z Allocation vector of the data to the mixture components

### Value

complete log-likelihood value

### Author(s)

 $\label{eq:complete} {\it Complete log-likelihood function for } q=0$ 

### Description

Complete log-likelihood function

### Usage

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

### **Arguments**

x\_data Data

w Mixture weightsmu Marginal means

SigmaINV Precision matrix (inverse covariance)

z Allocation vector of the data to the mixture components

#### Value

complete log-likelihood value

### Author(s)

Panagiotis Papastamoulis

complete.log.likelihood\_Sj

Complete log-likelihood function

### **Description**

Complete log-likelihood function

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

#### **Arguments**

x\_data Data

w Mixture weightsmu Marginal meansLambda Factor loadings

SigmaINV Precision matrix (inverse covariance) per component

z Allocation vector of the data to the mixture components

#### Value

complete log-likelihood value

### Author(s)

Panagiotis Papastamoulis

### **Description**

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

### Usage

```
\label{lem: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

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  $A, B, \Gamma, \Delta$  and a draw from the conditional distributions of  $\mu$  and  $\Lambda$ .

#### Author(s)

Panagiotis Papastamoulis

```
\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**

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

suff\_statistics

Sufficient statistics

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

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, B,  $\Gamma$ ,  $\Delta$  and a draw from the conditional distributions of  $\mu$  and  $\Lambda$ .

#### Author(s)

### 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**

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

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  $A, B, \Gamma, \Delta$  and a draw from the conditional distributions of  $\mu$  and  $\Lambda$ .

### Author(s)

Panagiotis Papastamoulis

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

#### Description

This function simulates  $\mu$ .

```
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

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

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  $A, B, \Gamma, \Delta$  and a draw from the conditional distributions of  $\mu$  and  $\Lambda$ .

#### 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

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

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  $A, B, \Gamma, \Delta$  and a draw from the conditional distributions of  $\mu$  and  $\Lambda$ .

#### Author(s)

Panagiotis Papastamoulis

```
\label{lem:compute_A_B_G_D_and_simulate_mu_Lambda_Sj} Computation\ and\ simulations
```

### 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, B,  $\Gamma$ ,  $\Delta$  and a draw from the conditional distributions of  $\mu$  and  $\Lambda$ .

#### Author(s)

compute\_sufficient\_statistics

Compute sufficient statistics

### Description

Compute sufficient statistics given y and z.

### Usage

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

### **Arguments**

 $\begin{array}{ll} y & Matrix \ of \ factors \\ z & Allocation \ vector \\ K & Number \ of \ components \\ x\_data & Data \end{array}$ 

## Value

A list with six entries of sufficient statistics.

### Author(s)

Panagiotis Papastamoulis

```
compute_sufficient_statistics_given_mu

Compute sufficient statistics given mu
```

### Description

Compute sufficient statistics given y and z.

### Usage

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

### **Arguments**

у	Matrix of factors
Z	Allocation vector
K	Number of components
x_data	Data

mu Means per component

### Value

A list with six entries of sufficient statistics.

### Author(s)

Panagiotis Papastamoulis

```
\label{eq:compute_sufficient_statistics_q0} Compute \ \textit{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.

### Author(s)

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.

 ${\tt compute\_regularized\_expression}$ 

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 15

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, 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**

model	Any subset of "UUU" "CUU" "UCU" "CCU" "UCC" "UUC" "CUC", "CCC" indicating the fitted models.
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 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.

bui ficycles	Number of cycles that will be discarded as built-in
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.

16 fabMix

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

proposing switchings. Default value: 5000.

over fitting Initialization

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

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 models.

All component-specific parameters have been reordered according to the ECR

algorithm in order to undo the label switching problem.

data The observed data.

#### Note

It is recommended to always 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.

### Author(s)

fabMix\_CxC

#### References

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

dealWithLabelSwitching

### **Examples**

```
## Not run:
# simulate a synthetic dataset along the lines of the paper:
                     # sample size
                     # number of variables
p = 40
q = 4
                    # number of factors
K = 10
                     # number of clusters
sINV_diag = 1/((1:p)) # diagonal of inverse variance of errors
set.seed(10)
syntheticDataset <- simData(K.true = K, n = n, q = q, p = p, sINV_values = sINV_diag )
# define parameters
Kmax <- 20 # number of overfitted mixture components
nChains <- 8 # number of parallel chains
dN < -1
# Dirichlet prior of mixture weights per chain.
   The target chain corresponds to the first entry.
dirPriorAlphas <- c(1, 1 + dN * (2:nChains - 1))/Kmax</pre>
outputFolder <- "fabMixExample"</pre>
# Run algorithm
fabMix( model = c("UUU" "CUU" "UCU" "CCU" "UCC" "UUC" "CUC", "CCC"),
dirPriorAlphas = dirPriorAlphas,
        rawData = syntheticDataset$data,
        outDir = outputFolder, Kmax = Kmax, mCycles = 1200,
        burnCycles = 200, q = 3:5)
## End(Not run)
```

fabMix\_CxC

Main function of the package for CUC, CCC models

### Description

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

18 fabMix\_CxC

#### 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.

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:  $\alpha=2$ . 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.

fabMix\_CxC

#### 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)

Panagiotis Papastamoulis

#### References

Papastamoulis, P. (2017). Overfitting Bayesian mixtures of factor analyzers with an unknown number of components. arXiv:1701.04605 [stat.ME]

#### See Also

dealWithLabelSwitching

#### **Examples**

```
## Not run:
# simulate a synthetic dataset along the lines of the paper:
n = 1000
                     # sample size
p = 40
                     # number of variables
q = 4
                     # number of factors
                      # number of clusters
K = 10
sINV_diag = 1/((1:p)) # diagonal of inverse variance of errors
syntheticDataset <- simData(K.true = K, n = n, q = q, p = p, sINV_values = sINV_diag )</pre>
# define parameters
Kmax <- 20 # number of overfitted mixture components
nChains <- 8 # number of parallel chains
dN < -1
# Dirichlet prior of mixture weights per chain.
    The target chain corresponds to the first entry.
dirPriorAlphas <- c(1, 1 + dN * (2:nChains - 1))/Kmax</pre>
outputFolder <- "fabMixExample"</pre>
# Run algorithm
fabMix_CxC( dirPriorAlphas = dirPriorAlphas,
        rawData = syntheticDataset$data,
        outDir = outputFolder, Kmax = Kmax, mCycles = 1200,
        burnCycles = 200, q = q)
# Compute information criteria:
#getStuffForDIC(x_data = syntheticDataset$data, outputFolder = outputFolder, q = q)
```

20 fabMix\_CxU

```
# Deal with label switching:
#dealWithLabelSwitching(x_data = syntheticDataset$data,
# outputFolder = outputFolder, q = q,
# compute_regularized_expression = TRUE, Km = Kmax)
## End(Not run)
```

fabMix\_CxU

Main function of the package for CCU, CUU models

#### **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**

- ·	T . 1 1			0 1	•
sameSigma	Logical value	denoting the	narameterization o	t the e	rror variance per compo-
Sallicatrilla	Logical value	uchoung mc	Darameterization o	ı uic ci	iroi variance dei combo-

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:  $\beta=1$ . fabMix\_CxU 21

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.

#### Author(s)

Panagiotis Papastamoulis

### References

Papastamoulis, P. (2017). Overfitting Bayesian mixtures of factor analyzers with an unknown number of components. arXiv:1701.04605 [stat.ME]

#### See Also

dealWithLabelSwitching

#### **Examples**

```
## Not run:
# simulate a synthetic dataset along the lines of the paper:
                     # sample size
p = 40
                     # number of variables
q = 4
                     # number of factors
K = 10
                      # number of clusters
sINV_diag = 1/((1:p)) # diagonal of inverse variance of errors
set.seed(10)
syntheticDataset <- simData(K.true = K, n = n, q = q, p = p, sINV_values = sINV_diag)
# define parameters
Kmax <- 20 # number of overfitted mixture components
nChains <- 8 # number of parallel chains
dN < -1
# Dirichlet prior of mixture weights per chain.
   The target chain corresponds to the first entry.
dirPriorAlphas <- c(1, 1 + dN * (2:nChains - 1))/Kmax
outputFolder <- "fabMixExample"</pre>
# Run algorithm
fabMix_CxU( dirPriorAlphas = dirPriorAlphas,
        rawData = syntheticDataset$data,
        outDir = outputFolder, Kmax = Kmax, mCycles = 1200,
        burnCycles = 200, q = q)
# Compute information criteria:
#getStuffForDIC(x_data = syntheticDataset$data, outputFolder = outputFolder, q = q)
# Deal with label switching:
#dealWithLabelSwitching(x_data = syntheticDataset$data,
         outputFolder = outputFolder, q = q,
         compute_regularized_expression = TRUE, Km = Kmax)
## End(Not run)
```

fabMix\_missing\_values Main function for the 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.

```
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 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. 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)

24  $fabMix\_UxC$ 

#### References

Papastamoulis, P. (2017). Overfitting Bayesian mixtures of factor analyzers with an unknown number of components. arXiv:1701.04605 [stat.ME]

#### See Also

```
dealWithLabelSwitching
```

#### **Examples**

```
## Not run:
# simulate a synthetic dataset along the lines of the paper:
n = 1000
                      # sample size
p = 40
                     # number of variables
q = 4
                     # number of factors
K = 10
                      # number of clusters
sINV_diag = 1/((1:p)) # diagonal of inverse variance of errors
set.seed(10)
syntheticDataset <- simData(K.true = K, n = n, q = q, p = p, sINV_values = sINV_diag)
# define parameters
Kmax <- 20 # number of overfitted mixture components
nChains <- 8 # number of parallel chains
dN <- 1
# Dirichlet prior of mixture weights per chain.
# The target chain corresponds to the first entry.
dirPriorAlphas <- c(1, 1 + dN * (2:nChains - 1))/Kmax
outputFolder <- "fabMixExample"</pre>
# Run algorithm
fabMix( dirPriorAlphas = dirPriorAlphas,
        rawData = syntheticDataset$data,
        outDir = outputFolder, Kmax = Kmax, mCycles = 1200,
        burnCycles = 200, q = q)
# Compute information criteria:
getStuffForDIC(x_data = syntheticDataset$data, outputFolder = outputFolder, q = q)
# Deal with label switching:
dealWithLabelSwitching(x_data = syntheticDataset$data,
        outputFolder = outputFolder, q = q,
        compute_regularized_expression = TRUE, Km = Kmax)
## End(Not run)
```

fabMix\_UxC 25

#### **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)
```

#### **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:  $\beta=1$ .

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.

26 fabMix\_UxC

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.

#### Author(s)

Panagiotis Papastamoulis

#### References

Papastamoulis, P. (2017). Overfitting Bayesian mixtures of factor analyzers with an unknown number of components. arXiv:1701.04605 [stat.ME]

#### See Also

dealWithLabelSwitching

### **Examples**

```
# simulate a synthetic dataset along the lines of the paper:
                     # sample size
                      # number of variables
p = 40
                     # number of factors
q = 4
K = 10
                      # number of clusters
sINV_diag = 1/((1:p)) # diagonal of inverse variance of errors
set.seed(10)
syntheticDataset < simData(K.true = K, n = n, q = q, p = p, sINV_values = sINV_diag)
# define parameters
Kmax <- 20 # number of overfitted mixture components
nChains <- 8 # number of parallel chains
dN < -1
# Dirichlet prior of mixture weights per chain.
    The target chain corresponds to the first entry.
dirPriorAlphas <- c(1, 1 + dN * (2:nChains - 1))/Kmax</pre>
outputFolder <- "fabMixExample"</pre>
```

fabMix\_UxU 27

fabMix\_UxU

Fit UxU mixtures

#### **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 of the error variance per component. 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 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.

28 fabMix\_UxU

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\_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.

#### Author(s)

Panagiotis Papastamoulis

#### References

Papastamoulis, P. (2017). Overfitting Bayesian mixtures of factor analyzers with an unknown number of components. arXiv:1701.04605 [stat.ME]

getStuffForDIC 29

### See Also

dealWithLabelSwitching

#### **Examples**

```
## Not run:
# simulate a synthetic dataset along the lines of the paper:
n = 1000
                    # sample size
p = 40
                     # number of variables
q = 4
                     # number of factors
K = 10
                      # number of clusters
sINV_diag = 1/((1:p)) # diagonal of inverse variance of errors
set.seed(10)
syntheticDataset < simData(K.true = K, n = n, q = q, p = p, sINV_values = sINV_diag)
# define parameters
Kmax <- 20 # number of overfitted mixture components
nChains <- 8 # number of parallel chains
dN <- 1
# Dirichlet prior of mixture weights per chain.
    The target chain corresponds to the first entry.
dirPriorAlphas <- c(1, 1 + dN * (2:nChains - 1))/Kmax
outputFolder <- "fabMixExample"
# Run algorithm
fabMix_UxU( dirPriorAlphas = dirPriorAlphas,
        rawData = syntheticDataset$data,
        outDir = outputFolder, Kmax = Kmax, mCycles = 1200,
        burnCycles = 200, q = q)
# Compute information criteria:
getStuffForDIC(x_data = syntheticDataset$data, outputFolder = outputFolder, q = q)
# Deal with label switching:
dealWithLabelSwitching(x_data = syntheticDataset$data,
        outputFolder = outputFolder, q = q,
        compute_regularized_expression = TRUE, Km = Kmax)
## End(Not run)
```

 ${\tt getStuffForDIC}$ 

Compute information criteria

### **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.

30 getStuffForDIC

### Usage

 $\label{eq:control} getStuffForDIC(sameSigma, sameLambda, isotropic, x\_data, outputFolder, q, burn, Km, normalize, discardLower)$ 

### 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

### **Details**

If necessary, more details than the description above

applied only for the DIC computation.

### Value

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

### 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.

### Author(s)

log\_dirichlet\_pdf 31

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)

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 Common covariance matrix of the errors per cluster

z Allocation vector

### Value

Log-likelihood value

### Author(s)

Panagiotis Papastamoulis

```
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.

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

#### **Arguments**

x\_data The observed data

w Vector of mixture weightsmu Vector of marginal means

Sigma Covariance matrix of the errors per cluster

z Allocation vector

#### Value

Log-likelihood value

### Author(s)

Panagiotis Papastamoulis

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 weightsmu Vector of marginal means

Lambda Factor loadings

Sigma Covariance matrix of the errors per cluster

z Allocation vector

### Value

Log-likelihood value

#### Author(s)

34 overfittingMFA

```
observed.log.likelihood0_Sj_q0  \label{eq:likelihood} \textit{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	Covariance matrix of the errors per cluster

z Allocation vector

#### Value

Log-likelihood value

### Author(s)

Panagiotis Papastamoulis

overfittingMFA Basic MCMC sampler

### Description

Gibbs sampling for fitting a mixture model of factor analyzers.

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

overfittingMFA\_CCC 35

#### **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

List of files

### Author(s)

Panagiotis Papastamoulis

overfittingMFA\_CCC

Basic MCMC sampler for CCC

#### **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 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:  $\beta=1$ .

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

gibbs\_z Optional

### Value

List of files

### Author(s)

Panagiotis Papastamoulis

overfittingMFA\_CCU

Basic MCMC sampler for CCU

#### **Description**

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

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

overfittingMFA\_CUC 37

#### **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:  $\beta=1$ .

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

gibbs\_z Optional

#### Value

List of files

# Author(s)

Panagiotis Papastamoulis

overfittingMFA\_CUC

Basic MCMC sampler for CUC

#### **Description**

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

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

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:  $\beta=1$ .

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

gibbs\_z Optional

#### Value

List of files

# Author(s)

Panagiotis Papastamoulis

overfittingMFA\_CUU

Basic MCMC sampler for CUU

#### **Description**

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

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

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)

Panagiotis Papastamoulis

overfittingMFA\_missing\_values

Basic MCMC sampler for the case of missing data

### Description

Gibbs sampling for fitting a mixture model of factor analyzers.

```
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)
```

40 overfittingMFA\_Sj

#### **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 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)

Panagiotis Papastamoulis

overfittingMFA\_Sj

Basic MCMC sampler using different error variance per component

### Description

Gibbs sampling for fitting a mixture model of factor analyzers.

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

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)

Panagiotis Papastamoulis

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.

```
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)
```

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 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)

Panagiotis Papastamoulis

overfittingMFA\_UCC

Basic MCMC sampler for CCC

### **Description**

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

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

overfittingMFA\_UUC 43

#### **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

List of files

### Author(s)

Panagiotis Papastamoulis

overfittingMFA\_UUC

Basic MCMC sampler for UUC

#### **Description**

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

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

44 overfitting\_q0

#### **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)

Panagiotis Papastamoulis

 $\label{eq:mcmc} \textit{overfitting\_q0} \qquad \qquad \textit{MCMC sampler for } q = 0$ 

# Description

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

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

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)

Panagiotis Papastamoulis

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.

```
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)
```

46 plot.fabMix.object

#### **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)

Panagiotis Papastamoulis

# Description

This function plots fabMix function.

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

print.fabMix.object 47

#### **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",

"regularized\_expression". 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 estimated regularized expression of each

variable to the factor space for the selected model, respectively.

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

... ignored.

#### **Details**

The function plots the BIC values obtained for each of the fitted models, visualizes the clusters.

#### Author(s)

Panagiotis Papastamoulis

#### **Description**

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

#### Usage

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

#### **Arguments**

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

printSubset Logical indicating whether to print the header or the whole matrix of estimates.

Default value: TRUE.

... ignored.

#### **Details**

The function prints the estimated distribution of the number of clusters, the estimated number of observations assigned to each cluster after post-processing the output with three label switching algorithms, as well as the header of the posterior mean estimates of  $\theta_{kj}$  (probability of success for cluster k and feature j) (conditionally on the most probable number of clusters).

#### Author(s)

48 simData

readLambdaValues

Read Lambda values.

# Description

Function to read Lambda values from file.

# Usage

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

# Arguments

myFile	File containing Lambda values
K	Number of components
р	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.

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

simData 49

#### **Arguments**

sameSigma Logical. sameLambda Logical.

p 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)).</pre>

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)

50 update\_all\_y\_Sj

update\_all\_y

Gibbs sampling for y

### **Description**

Gibbs sampling for y

### Usage

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

# **Arguments**

x\_data Data

mu Marginal means
SigmaINV Precision matrix
Lambda Factor loadings
z Allocation vector

# Value

A matrix with generated factors

### Author(s)

Panagiotis Papastamoulis

update\_all\_y\_Sj

Gibbs sampling for y

# Description

Gibbs sampling for y

# Usage

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

# Arguments

x\_data Data

mu Marginal means

SigmaINV Precision matrix per component

Lambda Factor loadings z Allocation vector

update\_OmegaINV 51

# Value

A matrix with generated factors

# Author(s)

Panagiotis Papastamoulis

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

 $\Omega^{-1}$ 

# Author(s)

update\_OmegaINV\_Cxx

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

# Description

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

# Usage

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

# Arguments

Lambda Factor loadings

K Number of components

g Prior parameterh Prior parameter

### Value

 $\Omega^{-1}$ 

### Author(s)

Panagiotis Papastamoulis

```
{\tt update\_SigmaINV\_faster}
```

Gibbs sampling for  $\Sigma^-1$ 

# Description

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

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

x\_data Data

z Allocation vector

y Factors

Lambda Factor loadings mu Marginal means

K Number of components

alpha\_sigma Prior parameter beta\_sigma Prior parameter

#### Value

 $\Sigma^{-1}$ 

### Author(s)

Panagiotis Papastamoulis

```
update_SigmaINV_faster_q0
```

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  $\Sigma^{-1}$  per component

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

x\_data Data

z Allocation vector

y Factors

Lambda Factor loadings mu Marginal means

K Number of components

alpha\_sigma Prior parameter beta\_sigma Prior parameter

#### Value

 $\Sigma^{-1}$ 

#### Author(s)

Panagiotis Papastamoulis

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 Data

z Allocation vector

y Factors

Lambda Factor loadings mu Marginal means

K Number of components

alpha\_sigma Prior parameter beta\_sigma Prior parameter

# Value

 $\Sigma^{-1}$ 

### Author(s)

Panagiotis Papastamoulis

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 Data

z Allocation vector

y Factors

Lambda Factor loadings
mu Marginal means

K Number of components

alpha\_sigma Prior parameter beta\_sigma Prior parameter

# Value

 $\Sigma^{-1}$ 

# Author(s)

update\_z2 57

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 Mixture weightsmu Marginal meansLambda Factor loadingsSigmaINV Precision matrix

K Number of components

x\_data Data

# Value

Allocation vector

# Author(s)

Panagiotis Papastamoulis

update\_z2\_Sj

Collapsed Gibbs for z using matrix inversion lemma

# Description

Collapsed Gibbs for z using matrix inversion lemma

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

58 update\_z4

#### **Arguments**

w Mixture weightsmu Marginal meansLambda Factor loadings

SigmaINV Precision matrix per component

K Number of components

x\_data Data

#### Value

Allocation vector

# Author(s)

Panagiotis Papastamoulis

update\_z4  $Collapsed\ Gibbs\ for\ z$ 

# Description

Collapsed Gibbs for z

# Usage

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

# Arguments

w Mixture weightsmu Marginal meansLambda Factor loadingsSigmaINV Precision matrix

K Number of components

x\_data Data

#### Value

Allocation vector

### Author(s)

update\_z4\_Sj 59

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 Mixture weightsmu Marginal meansLambda Factor loadings

SigmaINV Precision matrix per component

K Number of components

x\_data Data

# Value

Allocation vector

# Author(s)

Panagiotis Papastamoulis

update\_z\_b

Gibbs sampling for z

# Description

Gibbs sampling for z

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

60 update\_z\_b\_Sj

#### **Arguments**

w Mixture weightsmu Marginal meansLambda Factor loadingsy Matrix of factorsSigmaINV Precision matrix

K Number of components

x\_data Data

### Value

Allocation vector

# Author(s)

Panagiotis Papastamoulis

update\_z\_b\_Sj

Gibbs sampling for z

# Description

Gibbs sampling for z

# Usage

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

### **Arguments**

w Mixture weightsmu Marginal meansLambda Factor loadingsy Matrix of factors

SigmaINV Precision matrix per component

K Number of components

x\_data Data

#### Value

Allocation vector

# Author(s)

 $update\_z\_q0$  61

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 weightsmu Marginal means

SigmaINV Precision matrix per component

K Number of components

x\_data Data

# Value

Allocation vector

### Author(s)

Panagiotis Papastamoulis

```
update_z_q0_sameSigma Gibbs sampling for z for q = 0
```

# Description

Gibbs sampling for z

# Usage

```
update_z_q0_sameSigma(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

62 waveDataset1500

#### Value

Allocation vector

#### Author(s)

Panagiotis Papastamoulis

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 observa-

#### **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.

# **Index**

```
*Topic datasets
                                               myDirichlet, 31
    waveDataset1500, 62
                                               observed.log.likelihood0,32
*Topic package
                                               observed.log.likelihood0_q0_sameSigma,
    fabMix-package, 3
                                                        32
complete.log.likelihood,4
                                               observed.log.likelihood0_Sj,33
complete.log.likelihood_q0, 5
                                               observed.log.likelihood0_Sj_q0,34
complete.log.likelihood_q0_sameSigma,
                                               overfitting_q0,44
                                               overfitting_q0_sameSigma, 45
complete.log.likelihood_Sj,6
                                               overfittingMFA, 34
compute_A_B_G_D_and_simulate_mu_Lambda,
                                               overfittingMFA_CCC, 35
                                               overfittingMFA_CCU, 36
compute_A_B_G_D_and_simulate_mu_Lambda_CCU,
                                               overfittingMFA_CUC, 37
                                               overfittingMFA_CUU, 38
compute_A_B_G_D_and_simulate_mu_Lambda_CUU,
                                               overfittingMFA_missing_values, 39
                                               overfittingMFA_Sj, 40
compute_A_B_G_D_and_simulate_mu_Lambda_q0,
                                               overfittingMFA_Sj_missing_values, 41
                                               overfittingMFA_UCC, 42
compute_A_B_G_D_and_simulate_mu_Lambda_q0_samev@eigfinittingMFA_UUC, 43
                                               plot.fabMix.object, 4, 46
compute_A_B_G_D_and_simulate_mu_Lambda_Sj,
                                               print.fabMix.object, 47
compute_sufficient_statistics, 12
                                               readLambdaValues, 48
compute\_sufficient\_statistics\_given\_mu,
                                               simData, 48
compute_sufficient_statistics_q0, 13
                                               update_all_y, 50
dealWithLabelSwitching, 14, 17, 19, 21, 24,
                                               update_all_y_Sj, 50
        26, 29
                                               update_OmegaINV, 51
                                               update_OmegaINV_Cxx, 52
fabMix, 4, 15
                                               update_SigmaINV_faster, 52
fabMix-package, 3
                                               update_SigmaINV_faster_q0, 53
fabMix_CxC, 17
                                               update_SigmaINV_faster_q0_sameSigma,
fabMix_CxU, 20
                                                        54
fabMix_missing_values, 22
                                               update_SigmaINV_faster_Sj, 54
fabMix_UxC, 24
                                               update_SigmaINV_xCC, 55
fabMix_UxU, 27
                                               update_SigmaINV_xUC, 56
                                               update_z2, 57
getStuffForDIC, 29
                                               update_z2_Sj, 57
log_dirichlet_pdf, 31
                                               update_z4, 58
```

64 INDEX

```
update_z4_Sj, 59
update_z_b, 59
update_z_b_Sj, 60
update_z_q0, 61
update_z_q0_sameSigma, 61
waveDataset1500, 62
```