# Package 'fabMix'

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Type Package
<b>Title</b> Overfitting Bayesian Mixtures of Factor Analyzers with an Unknown Number of Components
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Model-based clustering of multivariate continuous data with or without missing values. The underlying model is a Bayesian mixture of factor analyzers with a large number of components (overfitting mixture). 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. Identifiability issues related to label switching are dealt by post-processing the simulated output with the ECR algorithm.  Imports MASS, doParallel, foreach, label.switching, mvtnorm, doRNG,
RColorBrewer, corrplot, mclust  License GPL-2
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## Description

fabMix-package

Model-based clustering of multivariate continuous data with or without missing values. The underlying model is a Bayesian mixture of factor analyzers with a large number of components (overfitting mixture). 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. Identifiability issues related to label switching are dealt by post-processing the simulated output with the ECR algorithm.

#### Author(s)

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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.

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

#### See Also

fabMix, dealWithLabelSwitching, getStuffForDIC

#### **Examples**

```
# 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 )</pre>
## Not run:
# 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)
```

complete.log.likelihood

Complete log-likelihood function

#### **Description**

Complete log-likelihood function

```
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 \ 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.

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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**

٤	Guments	
	model	Any subset of "UUU" "CUU" "UCU" "CCU" "UCC" "UUC" "CUC", "CCC" indicating the fitted models.
	${\tt dirPriorAlphas}$	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.
	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	A vector containing the number of factors to be fitted.
	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.

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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

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. (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</pre>
outputFolder <- "fabMixExample"</pre>
# Run algorithm
fabMix( dirPriorAlphas = dirPriorAlphas,
        rawData = syntheticDataset$data,
        outDir = outputFolder, Kmax = Kmax, mCycles = 1200,
        burnCycles = 200, q = q)
## 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.

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#### 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)
```

#### **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.

Prior parameter g. Default value: g = 2. g Prior parameter h. Default value: h = 1. Prior parameter  $\alpha$ . Default value:  $\alpha = 2$ . alpha\_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. Optional integer denoting the thinning of the keeped MCMC cycles. thinning

zStart Optional starting value for the allocation vector.

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

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

model. Default value: 1.

warm\_up\_overfitting

beta\_sigma

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

100.

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

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.

Initialization parameter. Default: 0.05. gwar

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)
# 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)
```

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```
# 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 er	ror variance per compo-
Sallicatrilla	Logical value	uchoung mc	Darameterization o	n une en	101 variance bei 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)

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#### 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)
```

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#### **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.

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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>
```

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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.

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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.

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## 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)

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```
observed.log.likelihood0_Sj_q0  {\it 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)
```

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#### **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, ...)
```

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.

... 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

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**

Logical. sameSigma sameLambda Logical. The dimension of the multivariate normal distribution (p > 1). Number of factors. It should be strictly smaller than p. q K.true The number of mixture components (clusters). 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 $k=1,\ldots,K; r=1,\ldots,p; j=1,\ldots,q$ .
means	$K.true \times p$ matrix containing the marginal means $\mu_{kr}, \ k=1,\ldots,K; \ r=1,\ldots,p.$
variance	$p \times p$ diagonal matrix containing the variance of errors $\sigma_{rr}$ , $r=1,\ldots,p$ . 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.

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# Note

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

# Author(s)

Panagiotis Papastamoulis

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)

50 update\_OmegaINV

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

#### 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
i allibua	Factor toadings

K Number of components

g Prior parameterh Prior parameter

# Value

 $\Omega^{-1}$ 

### Author(s)

Panagiotis Papastamoulis

update\_SigmaINV\_faster

Gibbs sampling for  $\Sigma^-1$ 

# Description

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

# Usage

```
update_SigmaINV_faster(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)

### **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)

Panagiotis Papastamoulis

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

# Description

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

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

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

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

### **Description**

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

# Usage

```
update_SigmaINV_faster_Sj(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\_SigmaINV\_xCC G

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

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

update\_z2 55

### **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\_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)

56 update\_z4

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 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  $\boldsymbol{z}$ 

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

update\_z4\_Sj 57

### **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\_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)

58 update\_z\_b\_Sj

update\_z\_b

Gibbs sampling for z

# Description

Gibbs sampling for z

### Usage

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

### **Arguments**

w Mixture weights
 mu Marginal means
 Lambda Factor loadings
 y Matrix of factors
 SigmaINV 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

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

 $update\_z\_q0$  59

# **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)

Panagiotis Papastamoulis

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)

60 waveDataset1500

```
\mbox{update\_z\_q0\_sameSigma} \ \ \mbox{\it 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 weightsmu Marginal means

SigmaINV Precision matrix per component

K Number of components

x\_data Data

#### Value

Allocation vector

#### Author(s)

Panagiotis Papastamoulis

waveDataset1500	Wave dataset
WaveDataSet1300	wave aaiasei

#### **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.

waveDataset1500 61

### 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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