Package 'fabMix'

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Type Package

| Title 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 switch ing are dealt by post-processing the simulated output with the ECR algorithm. |
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| fabMix-package complete.log.likelihood complete.log.likelihood_q0 complete.log.likelihood_q0_sameSigma complete.log.likelihood_Sj compute_A_B_G_D_and_simulate_mu_Lambda compute_A_B_G_D_and_simulate_mu_Lambda_CCU compute_A_B_G_D_and_simulate_mu_Lambda_CUU |

compute_A_B_G_D_and_simulate_mu_Lambda_q09compute_A_B_G_D_and_simulate_mu_Lambda_q0_sameSigma10compute_A_B_G_D_and_simulate_mu_Lambda_Sj11

2

Index

| compute_sufficient_statistics | 12 |
|--|----|
| compute_sufficient_statistics_given_mu | 12 |
| compute_sufficient_statistics_q0 | 13 |
| dealWithLabelSwitching | 14 |
| fabMix | 15 |
| fabMix_CxU | 17 |
| fabMix_missing_values | 19 |
| getStuffForDIC | 22 |
| log_dirichlet_pdf | 23 |
| myDirichlet | 24 |
| observed.log.likelihood0 | 24 |
| observed.log.likelihood0_q0_sameSigma | 25 |
| observed.log.likelihood0_Sj | 26 |
| observed.log.likelihood0_Sj_q0 | 26 |
| overfittingMFA | 27 |
| overfittingMFA_CCU | 28 |
| overfittingMFA_CUU | 29 |
| overfittingMFA_missing_values | 30 |
| overfittingMFA_Sj | 31 |
| overfittingMFA_Sj_missing_values | 32 |
| overfitting_q0 | 33 |
| overfitting_q0_sameSigma | 34 |
| simData | 35 |
| update_all_y | 36 |
| update_all_y_Sj | 37 |
| update_OmegaINV | 37 |
| update_SigmaINV_faster | 38 |
| update_SigmaINV_faster_q0 | 39 |
| update_SigmaINV_faster_q0_sameSigma | 39 |
| update_SigmaINV_faster_Sj | 40 |
| update_z2 | 41 |
| update_z2_Sj | 41 |
| update_z4 | 42 |
| update_z4_Sj | 43 |
| update_z_b | 43 |
| update_z_b_Sj | 44 |
| update_z_q0 | 45 |
| update_z_q0_sameSigma | 45 |
| waveDataset1500 | 46 |
| | |
| | 47 |

fabMix-package 3

| fabMix-package | Overfitting Bayesian Mixtures of Factor Analyzers with an Unknown Number of Components |
|-----------------|--|
| Tabii1X-package | |

Description

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 Learning, 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: 

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 )</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

Usage

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

Arguments

x_dataDataw Mixture weightsmu Marginal means

Lambda 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 weights

mu 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

Usage

```
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 μ and Λ .

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 Σ^{-1}

suff_statistics

Sufficient statistics

OmegaINV Prior parameter: Ω^{-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, Γ, Δ and a draw from the conditional distributions of μ and Λ .

Author(s)

Panagiotis Papastamoulis

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

Description

This function simulates μ and Λ 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 Σ^{-1}

suff_statistics

Sufficient statistics

OmegaINV Prior parameter: Ω^{-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, Γ , Δ and a draw from the conditional distributions of μ and Λ .

Author(s)

Description

This function simulates μ and Λ 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 Σ^{-1}

suff_statistics

Sufficient statistics

OmegaINV Prior parameter: Ω^{-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, Γ, Δ and a draw from the conditional distributions of μ and Λ .

Author(s)

Panagiotis Papastamoulis

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

Description

This function simulates μ .

Usage

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

Arguments

SigmaINV Precision matrix Σ^{-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, Γ, Δ and a draw from the conditional distributions of μ and Λ .

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 μ .

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 Σ^{-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, Γ, Δ and a draw from the conditional distributions of μ and Λ .

Author(s)

Panagiotis Papastamoulis

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

Description

This function simulates μ and Λ .

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 Σ^{-1} per component

suff_statistics

Sufficient statistics

OmegaINV Prior parameter: Ω^{-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, Γ , Δ and a draw from the conditional distributions of μ and Λ .

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.

fabMix 15

|--|

Description

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

Usage

```
fabMix(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

gibbs_z

| ě | guments | |
|---|----------------|--|
| | 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. |
| | g | Prior parameter g . Default value: $g = 2$. |
| | h | Prior parameter h . Default value: $h = 1$. |
| | alpha_sigma | Prior parameter α . Default value: $\alpha = 2$. |
| | beta_sigma | Prior parameter β . Default value: $\beta = 1$. |
| | q | Number of factors q , where $1 \leq q \leq L$. 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. |
| | | |

model. Default value: 1.

Select the gibbs sampling scheme for updating latent allocations of mixture

16 fabMix

```
warm_up_overfitting
```

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

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

fabMix_CxU

```
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$data,
        outDir = outputFolder, Kmax = Kmax, mCycles = 1200,
        burnCycles = 200, q = q)
# Compute information criteria:
getStuffForDIC(x_data = syntheticDataset$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_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

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.

 $fabMix_CxU$

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 α . Default value: $\alpha=2$. beta_sigma Prior parameter β . 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)

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_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)
```

Description

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

Usage

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

Arguments

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

nent. If 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 α . Default value: $\alpha=2$. beta_sigma Prior parameter β . 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 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)

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
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)
```

22 getStuffForDIC

getStuffForDIC

Compute information criteria

Description

This function computes four information criteria for a given run of the fabMix algorithm, namely: AIC, BIC, DIC and DIC₂. Given various runs with different number of factors, the selected model corresponds to the one with the smalled value of the selected criterion.

Usage

```
getStuffForDIC(sameSigma, sameLambda, 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. |
| x_data | Observed data. |
| outputFolder | Name of the folder where the fabMix function has saved its output. |
| q | Number of factors. Note that this should coincide with the number of factors in the fabMix run. |
| burn | Discard observations as burn-in period (optional). |
| Km | Number of components in the overfitted mixture model. Note that this should coincide with the same entry in the fabMix run. |
| normalize | Should the observed data be normalized? Note that this should coincide with the same entry in the fabMix run. Default value: TRUE. |
| discardLower | Discard draws with log-likelihood values lower than the specific quantile. This applied only for the DIC computation. |

Details

If necessary, more details than the description above

log_dirichlet_pdf 23

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)

Panagiotis Papastamoulis

log_dirichlet_pdf

Log-density function of the Dirichlet distribution

Description

Log-density function of the Dirichlet distribution

Usage

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

Arguments

alpha Parameter vector weights Vector of weights

Value

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

Author(s)

myDirichlet

Simulate from the Dirichlet distribution

Description

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

Usage

```
myDirichlet(alpha)
```

Arguments

alpha

Parameter vector

Value

Simulated vector

Author(s)

Panagiotis Papastamoulis

observed.log.likelihood0

Log-likelihood of the mixture model

Description

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

Usage

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

Arguments

x_data The observed data

w Vector of mixture weights mu 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.

Usage

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

Arguments

| x_data | The observed | data |
|--------|--------------|------|
| | | |

w Vector of mixture weights
mu Vector of marginal means

Sigma Covariance matrix of the errors per cluster

z Allocation vector

Value

Log-likelihood value

Author(s)

```
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

| v | data | The observed data |
|---|------|--------------------|
| х | uata | i ne 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)

Panagiotis Papastamoulis

```
observed.log.likelihood0\_Sj\_q0
```

Log-likelihood of the mixture model for q = 0

Description

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

Usage

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

overfittingMFA 27

Arguments

x_dataThe observed dataWVector 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.

Usage

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

Arguments

x_data normalized data

originalX observed raw data (only for plotting purpose)

outputDirectory

Name of the output folder

Kmax Number of mixture components

m Number of iterationsthinning Thinning of chainburn Burn-in period

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

alpha_prior Parameters of the Dirichlet prior distribution of mixture weights.

alpha_sigma Prior parameter α . Default value: $\alpha=2$. beta_sigma Prior parameter β . 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.

Usage

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

Arguments

x_data normalized data

originalX observed raw data (only for plotting purpose)

outputDirectory

Name of the output folder

Kmax Number of mixture components

m Number of iterationsthinning Thinning of chainburn Burn-in period

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

alpha_prior Parameters of the Dirichlet prior distribution of mixture weights.

alpha_sigma Prior parameter α . Default value: $\alpha=2$. beta_sigma Prior parameter β . Default value: $\beta=1$.

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

gibbs_z Optional

overfittingMFA_CUU 29

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.

Usage

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

Arguments

x_data normalized data

originalX observed raw data (only for plotting purpose)

outputDirectory

Name of the output folder

Kmax Number of mixture components

m Number of iterationsthinning Thinning of chainburn Burn-in period

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

alpha_prior Parameters of the Dirichlet prior distribution of mixture weights.

alpha_sigma Prior parameter α . Default value: $\alpha=2$. beta_sigma Prior parameter β . 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.

Usage

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

Arguments

missing_entries

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

entries) for every row containing missing values.

x_data normalized data

originalX observed raw data (only for plotting purpose)

outputDirectory

Name of the output folder

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 α . Default value: $\alpha=2$. beta_sigma Prior parameter β . Default value: $\beta=1$.

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

gibbs_z Optional

Value

List of files

overfittingMFA_Sj 31

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.

Usage

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

Arguments

x_data normalized data

originalX observed raw data (only for plotting purpose)

outputDirectory

Name of the output folder

Kmax Number of mixture components

m Number of 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 α . Default value: $\alpha=2$. beta_sigma Prior parameter β . 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)

```
overfittingMFA_Sj_missing_values
```

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

Description

Gibbs sampling for fitting a mixture model of factor analyzers.

Usage

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

Arguments

missing_entries

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

entries) for every row containing missing values.

x_data normalized data

originalX observed raw data (only for plotting purpose)

outputDirectory

Name of the output folder

Kmax Number of mixture components

m Number of iterationsthinning Thinning of chainburn Burn-in period

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

alpha_prior Parameters of the Dirichlet prior distribution of mixture weights.

alpha_sigma Prior parameter α . Default value: $\alpha=2$. beta_sigma Prior parameter β . Default value: $\beta=1$.

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

gibbs_z Optional

Value

List of files

overfitting_q0 33

Author(s)

Panagiotis Papastamoulis

overfitting_q0 MCMC sampler for q=0

Description

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

Usage

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

Arguments

x_data normalized data

originalX observed raw data (only for plotting purpose)

outputDirectory

Name of the output folder

Kmax Number of mixture components

m Number of iterationsthinning Thinning of 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 α . Default value: $\alpha=2$. beta_sigma Prior parameter β . Default value: $\beta=1$.

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

gibbs_z Optional

Value

List of files

Author(s)

```
overfitting_q0_sameSigma
```

MCMC sampler for q = 0 and same error variance parameterization

Description

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

Usage

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

Arguments

x_data normalized data

originalX observed raw data (only for plotting purpose)

outputDirectory

Name of the output folder

Kmax Number of mixture components

m Number of iterationsthinning Thinning of chainburn Burn-in period

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

alpha_prior Parameters of the Dirichlet prior distribution of mixture weights.

alpha_sigma Prior parameter α . Default value: $\alpha=2$. beta_sigma Prior parameter β . 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)

simData 35

| simData Synthetic data generator | |
|----------------------------------|--|
|----------------------------------|--|

Description

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

Usage

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

Arguments

sameSigma Logical. sameLambda Logical. 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 Λ_{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 $\mu_{kr}, k = 1, \dots, K; r =$ |
| | $1,\ldots,p$. |
| variance | $p \times p$ diagonal matrix containing the variance of errors σ_{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. |

36 update_all_y

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)

update_all_y_Sj 37

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 Ω^-1

Description

Gibbs sampling for Ω^{-1}

Usage

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

Arguments

| | - 1 11 |
|--------|-----------------|
| Lambda | Factor loadings |

K Number of components

g Prior parameterh Prior parameter

Value

 Ω^{-1}

Author(s)

Panagiotis Papastamoulis

update_SigmaINV_faster

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

Description

Gibbs sampling for Σ^{-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

 Σ^{-1}

Author(s)

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

Description

Gibbs sampling for Σ^{-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

 Σ^{-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 Σ^{-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

 Σ^{-1}

Author(s)

Panagiotis Papastamoulis

update_SigmaINV_faster_Sj

Gibbs sampling for Σ^-1 per component

Description

Gibbs sampling for Σ^{-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

 Σ^{-1}

Author(s)

update_z2 41

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

Usage

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

42 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 43

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

Usage

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

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)

 $update_z_q0$ 45

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

46 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

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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
                                                   observed.log.likelihood0_q0_sameSigma,
    waveDataset1500, 46
*Topic package
                                                   observed.log.likelihood0_Sj, 26
    fabMix-package, 3
                                                   observed.log.likelihood0_Sj_q0,26
                                                   overfitting_q0, 33
complete.log.likelihood,4
                                                   overfitting_q0_sameSigma, 34
complete.log.likelihood_q0,5
                                                   overfittingMFA, 27
complete.log.likelihood_q0_sameSigma,
                                                   overfittingMFA_CCU, 28
                                                   overfittingMFA_CUU, 29
complete.log.likelihood_Sj, 6
                                                   overfittingMFA_missing_values, 30
compute\_A\_B\_G\_D\_and\_simulate\_mu\_Lambda,
                                                   overfittingMFA_Sj, 31
                                                   overfittingMFA_Sj_missing_values, 32
compute\_A\_B\_G\_D\_and\_simulate\_mu\_Lambda\_CCU,
                                                   simData, 35
compute_A_B_G_D_and_simulate_mu_Lambda_CUU,
                                                   update_all_y, 36
                                                   update_all_y_Sj, 37
compute\_A\_B\_G\_D\_and\_simulate\_mu\_Lambda\_q0,
                                                   update_OmegaINV, 37
\verb|compute_A_B_G_D_and_simulate_mu_Lambda_q0_sam| \textit{esg} \textit{pha}_s SigmaINV\_faster, \textit{38} \\
                                                   update_SigmaINV_faster_q0,39
                                                   update_SigmaINV_faster_q0_sameSigma,
compute_A_B_G_D_and_simulate_mu_Lambda_Sj,
                                                   update_SigmaINV_faster_Sj, 40
compute_sufficient_statistics, 12
                                                   update_z2, 41
compute_sufficient_statistics_given_mu,
                                                   update_z2_Sj, 41
                                                   update_z4, 42
compute_sufficient_statistics_q0, 13
                                                   update_z4_Sj, 43
{\tt dealWithLabelSwitching}, \textit{3}, \textit{14}, \textit{16}, \textit{19}, \textit{21}
                                                   update_z_b, 43
                                                   update_z_b_Sj, 44
fabMix, 3, 15
                                                   update_z_q0, 45
fabMix-package, 3
                                                   update_z_q0_sameSigma, 45
fabMix_CxU, 17
                                                   waveDataset1500, 46
fabMix_missing_values, 19
getStuffForDIC, 3, 22
log_dirichlet_pdf, 23
myDirichlet, 24
observed.log.likelihood0,24
```