Package 'fabMix'

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Type Package

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

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Maintainer Panagiotis Papastamoulis <papapast@yahoo.gr>

Description

Model-based clustering of multivariate continuous data using Bayesian mixtures of factor analyzers (Papastamoulis, 2018 Computational Statistics and Data Analysis). The number of clusters is estimated using overfitting mixture models (Rousseau and Mengersen, 2011 Journal of the Royal Statistical Society B): suitable prior assumptions ensure that asymptotically the extra components will have zero posterior weight, therefore, the inference is based on the ``alive" components. A Gibbs sampler is implemented in order to (approximately) sample from the posterior distribution of the overfitting mixture. A prior parallel tempering scheme is also available, which allows to run multiple parallel chains with different prior distributions on the mixture weights. These chains run in parallel and can swap states using a Metropolis-Hastings move. Eight different parameterizations give rise to parsimonious representations of the covariance per cluster (following Mc Nicholas and others, 2008 Statistics and Computing). The model parameterization and number of factors is selected according to the Bayesian Information Criterion. Identifiability issues related to label switching are dealt by post-processing the simulated output with the Equivalence Classes Representatives algorithm (Papastamoulis 2010 Journal of Computational and Graphical Statistics, 2016 Journal of Statistical Software). Missing values are currently allowed for two model parameterizations.

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

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

LinkingTo Rcpp, RcppArmadillo

NeedsCompilation yes

Author Panagiotis Papastamoulis [aut, cre] (0000-0001-9468-7613)

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Description

Model-based clustering of multivariate continuous data using Bayesian mixtures of factor analyzers (Papastamoulis, 2018 Computational Statistics and Data Analysis). The number of clusters is estimated using overfitting mixture models (Rousseau and Mengersen, 2011 Journal of the Royal Statistical Society B): suitable prior assumptions ensure that asymptotically the extra components will have zero posterior weight, therefore, the inference is based on the "alive" components. A Gibbs sampler is implemented in order to (approximately) sample from the posterior distribution of the overfitting mixture. A prior parallel tempering scheme is also available, which allows to run multiple parallel chains with different prior distributions on the mixture weights. These chains run in parallel and can swap states using a Metropolis-Hastings move. Eight different parameterizations give rise to parsimonious representations of the covariance per cluster (following Mc Nicholas and others, 2008 Statistics and Computing). The model parameterization and number of factors is selected according to the Bayesian Information Criterion. Identifiability issues related to label switching are dealt by post-processing the simulated output with the Equivalence Classes Representatives algorithm (Papastamoulis 2010 Journal of Computational and Graphical Statistics, 2016 Journal of Statistical Software). Missing values are currently allowed for two model parameterizations.

Covariance and Unknown Number of Components

The main fuction of the package is fabMix.

Author(s)

Panagiotis Papastamoulis

Maintainer: Panagiotis Papastamoulis <papapast@yahoo.gr>

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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.

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

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

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

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

See Also

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

Examples

```
# TOY EXAMPLE (very small numbers... only for CRAN check purposes)
# (a) using 2 cores in parallel, each one running 2 heated chains.
library('fabMix')
n = 8
                  # sample size
p = 5
                  # number of variables
q = 2
                  # number of factors
K = 2
         # true number of clusters
sINV_{diag} = 1/((1:p)) # diagonal of inverse variance of errors
set.seed(100)
syntheticDataset <- simData(sameLambda=TRUE, K.true = K, n = n, q = q, p = p,
sINV_values = sINV_diag)
colnames(syntheticDataset$data) <- paste0("x_",1:p)</pre>
# Run `fabMix` for a _small_ number of iterations for the
# `UUU` (maximal model) and `CCC` (minimal model) parameterizations,
# using the default prior parallel heating parameters `dirPriorAlphas`.
# NOTE: `dirPriorAlphas` may require some tuning in general.
qRange <- 2 # values for the number of factors (only the true number
```

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

```
## 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_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)

Panagiotis Papastamoulis

```
complete.log.likelihood\_q0\_sameSigma
```

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)

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

v	_data	Data
Х_	_uata	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

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

Description

This function simulates μ and Λ .

Usage

```
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

OmegaINV

Sufficient statistics
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_AB_GD_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

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

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_A_B_G_D_and_simulate_mu_Lambda_CUU} Computation\ and\ simulations\ for\ CUU
```

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

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)

```
\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

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

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_A_B_G_D_and_simulate_mu_Lambda_q0_sameSigma} Computation\ and\ simulations\ for\ q=0.
```

Description

This function simulates μ .

Usage

```
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

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

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

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

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)

Panagiotis Papastamoulis

compute_sufficient_statistics

Compute sufficient statistics

Description

Compute sufficient statistics given y and z.

Usage

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

Arguments

y Matrix of factors

z Allocation vector

K Number of components

x_data Data

Value

A list with six entries of sufficient statistics.

Author(s)

```
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

y 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

dealWithLabelSwitching

Value

A list with six entries of sufficient statistics.

Author(s)

Panagiotis Papastamoulis

dealWithLabelSwitching

Apply label switching algorithms

Description

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

Usage

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

Arguments

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

ance per cluster is used.

x_data Data

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

q Number of factors

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

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

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

rameter values in simulated data.

compute_regularized_expression

Logical. Should regularized expression be computed?

Km Number of components in the overfitted mixture model.

Value

The following files are produced in the output folder:

Author(s)

Panagiotis Papastamoulis

References

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

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

Arguments

model	Any subset of "UUU" "CUU" "UCU" "CCU" "UCC" "UUC" "CUC", "CCC" indicating the fitted models. By default, all models are fitted.
nChains	The number of parallel heated chains. When 'dirPriorAlphas' is supplied, 'nChains' can be ignored.
dirPriorAlphas	vector of length nChains in the form of an increasing sequence of positive scalars. Each entry contains the (common) prior Dirichlet parameter for the corresponding chain. Default: $dirPriorAlphas = c(1, 1 + dN*(2:nChains - 1))/Kmax$, where $dN = 1$, for nChains > 1. Otherwise, $dirPriorAlphas = 1/Kmax$.
rawData	The observed data as an $n \times p$ matrix. Clustering is performed on the rows of the matrix.
outDir	Name of the output folder. An error is thrown if the directory already exists inside the current working directory. Note: it should NOT correspond to an absolute path, e.g.: outDir = `fabMix_example` is acceptable, but outDir = `C:\Username\Documents\fabMix_example` is not.
Kmax	Number of components in the overfitted mixture. Default: 20.
mCycles	Number of MCMC cycles. Each cycle consists of nIterPerCycle MCMC iterations. At the end of each cycle a swap of the state of two randomly chosen adjacent chains is attempted.
burnCycles	Number of cycles that will be discarded as burn-in period.
g	Prior parameter g . Default value: $g = 0.5$.
h	Prior parameter h . Default value: $h = 0.5$.
alpha_sigma	Prior parameter α . Default value: $\alpha = 0.5$.
beta_sigma	Prior parameter β . Default value: $\beta = 0.5$.
q	A vector containing the number of factors to be fitted.
normalize	Should the observed data be normalized? Default value: TRUE. (Recommended)

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

zStart Optional starting value for the allocation vector.

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

gibbs_z Select the gibbs sampling scheme for updating latent allocations of mixture

model. Default value: 1.

warm_up_overfitting

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

500.

warm_up Number of iterations that will be used to initialize the models before starting

proposing switchings. Default value: 5000.

overfittingInitialization

Logical value indicating whether the chains are initialized via the overfitting

initialization scheme. Default: TRUE.

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

sampler runs. Default: FALSE.

gwar Initialization parameter. Default: 0.05.

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

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

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

NULL (no model-level parallelization).

Details

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

UUU model: $(X_i|Z_i=k) = \mu_k + \Lambda_k Y_i + \varepsilon_i$, with $\varepsilon_i \sim \mathcal{N}(0, \Sigma_k)$

UCU model: $(X_i|Z_i=k) = \mu_k + \Lambda_k Y_i + \varepsilon_i$, with $\varepsilon_i \sim \mathcal{N}(0, \Sigma)$

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

UCC model: $(\mathbf{X}_i|Z_i=k)=\boldsymbol{\mu}_k+\boldsymbol{\Lambda}_k\mathbf{Y}_i+\boldsymbol{\varepsilon}_i$, with $\boldsymbol{\varepsilon}_i\sim\mathcal{N}(0,\sigma\mathbf{I}_p)$

CUU model: $(X_i|Z_i=k) = \mu_k + \Lambda Y_i + \varepsilon_i$, with $\varepsilon_i \sim \mathcal{N}(0, \Sigma_k)$

CCU model: $(X_i|Z_i=k) = \mu_k + \Lambda Y_i + \varepsilon_i$, with $\varepsilon_i \sim \mathcal{N}(0, \Sigma)$

CUC model: $(\mathbf{X}_i|Z_i=k)=\boldsymbol{\mu}_k+\boldsymbol{\Lambda}\mathbf{Y}_i+\boldsymbol{\varepsilon}_i$, with $\boldsymbol{\varepsilon}_i\sim\mathcal{N}(0,\sigma_k\mathbf{I}_p)$

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

In all cases, ε_i and Y_i are assumed independent, $i=1,\ldots,n$. Note that Σ_k and Σ denote positive definite matrices, I_p denotes the $p \times p$ identity matrix and σ_k , σ denote positive scalars.

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Value

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

bic Bayesian Information Criterion per model and number of factors.

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

model.

n_Clusters_per_model

The most probable number of clusters (number of non-empty components of the overfitted mixture) per model and number of factors.

posterior_probability

The posterior probability of the estimated allocations according to the selected

model.

covariance_matrix

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

the selected model.

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

model.

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

lected model.

selected_model

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

the selected model.

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

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

identifiable due to sign-switching across the MCMC trace.

data The observed data.

Note

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

Parallelization is enabled in both the chain-level as well as the model-level. By default all heated chains (specified by the nchains argument) run in parallel using (at most) the same number of threads (if available). If parallelModels = NULL (default), then the selected parameterizations will run (serially) on the same thread. Otherwise, if parallelModels = x (where x denotes a positive integer), the algorithm will first use x threads to fit the specified model parameterizations in parallel, and furthermore will also parallelize the heated chains (according to the remaining free cores on the user's system). The user should combine parallelModels with nChains efficiently, for example: if the number of available threads equals 12 and the user wishes to run 3 heated chains per model (recall that there are 8 parameterizations in total), then, an ideal allocation would be parallelModels = 4 and nChains = 3 because all available threads will be constantly

fabMix 19

busy. If the user wishes to run nChains = 4 heated chains per model using 12 threads, then an ideal allocation would be parallelModels = 3 models running in parallel. In the case where parallelModels*nChains>m, with m denoting the available number of threads, the algorithm will first allocate min(parallelModels, m) threads to run the same number of parameterizations in parallel, and then the remaining threads (if any) will be used to process the parallel heated chains. If no other threads are available, the heated chains will be allocated to single threads.

Author(s)

Panagiotis Papastamoulis

References

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

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

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

See Also

```
plot.fabMix.object
```

Examples

```
# (b) using 12 cores_
#_____4 models with 3 heated chains running in parallel______
#_____considering all 8 model parameterizations_____
## Not run:
library('fabMix')
set.seed(99)
n = 200
                    # sample size
p = 30
                   # number of variables
                  # number of factors
q = 2
K = 5
         # number of clusters
sINV_{diag} = rep(1/20,p) # diagonal of inverse variance of errors
syntheticDataset <- simData(sameLambda=FALSE,K.true = K, n = n, q = q, p = p,
sINV_values = sINV_diag)
colnames(syntheticDataset$data) <- paste0("x_",1:p)</pre>
qRange <- 1:3 # range of values for the number of factors
Kmax <- 20 # number of components for the overfitted mixture model
nChains <- 3 # number of parallel heated chains
# the next command takes ~ 2 hours in a Linux machine with 12 threads.
fm <- fabMix( parallelModels = 4,</pre>
nChains = nChains,
model = c("UUU", "CUU", "UCU", "CCU", "UCC", "UUC", "CUC", "CCC"),
```

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fabMix CxC

Function to estimate the CUC and CCC models

Description

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

Usage

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

Arguments

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

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

tion CUU is fitted.

dirPriorAlphas The prior Dirichlet parameters for each chain.

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

the matrix.

outDir Name of the output folder.

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

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

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

adjacent chains is attempted.

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. fabMix_CxC 21

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_overfitting

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

100.

warm_up Number of iterations that will be used to initialize the models before starting

proposing switchings. Default value: 500.

overfittingInitialization

Logical value indicating whether the chains are initialized via the overfitting

initialization scheme. Default: TRUE.

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

sampler runs. Default: FALSE.

gwar Initialization parameter. Default: 0.05.

cccStart Initialization from the CCC model.

Value

List of files written to outDir

Note

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

Author(s)

Panagiotis Papastamoulis

See Also

fabMix

22 $fabMix_CxU$

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Function to estimate the CCU and 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.

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_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

See Also

fabMix

 $\begin{array}{ll} {\sf fabMix_missing_values} & \textit{Function to estimate the UUU or UCU models in case of missing values} \\ & \textit{ues} \end{array}$

Description

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

Usage

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

Arguments

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

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

UUU model is fitted.

dirPriorAlphas The prior Dirichlet parameters for each chain.

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

the matrix.

outDir Name of the output folder.

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

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

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

adjacent chains is attempted.

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

g Prior parameter g. Default value: g=2. h Prior parameter h. Default value: h=1. alpha_sigma Prior parameter 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 NUmber of iterations that will be used to initialize the models before starting

proposing switchings. Default value: 500.

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

sampler runs. Default: FALSE.

gwar Initialization parameter. Default: 0.05.

Value

List of files written to outDir

Note

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

Author(s)

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

Description

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

Usage

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

Arguments

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

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

warm_up_overfitting

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

500.

warm_up Number of iterations that will be used to initialize the models before starting

proposing switchings. Default value: 5000.

overfittingInitialization

Logical value indicating whether the chains are initialized via the overfitting

initialization scheme. Default: TRUE.

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

sampler runs. Default: FALSE.

gwar Initialization parameter. Default: 0.05.

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

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

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

Value

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

Author(s)

Panagiotis Papastamoulis

fabMix_UxC

Function to estimate the UUC and UCC models

Description

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

Usage

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

fabMix_UxC 27

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 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

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Note

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

Author(s)

Panagiotis Papastamoulis

See Also

fabMix

fabMix_UxU

Function to estimate the UUU and UCU model

Description

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

Usage

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

Arguments

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

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

dirPriorAlphas The prior Dirichlet parameters for each chain.

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

the matrix.

outDir Name of the output folder.

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

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

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

adjacent chains is attempted.

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

g Prior parameter g. Default value: g=2. h Prior parameter h. Default value: h=1. fabMix_UxU 29

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)

Panagiotis Papastamoulis

See Also

fabMix

30 getStuffForDIC

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

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

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 applied only for the DIC computation.

Details

If necessary, more details than the description above

Value

The information criteria are saved to the informationCriteria_map_model.txt file in the code-outputFolder.

log_dirichlet_pdf 31

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)

Panagiotis Papastamoulis

myDirichlet

Simulate from the Dirichlet distribution

Description

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

Usage

```
myDirichlet(alpha)
```

Arguments

alpha

Parameter vector

Value

Simulated vector

Author(s)

Panagiotis Papastamoulis

observed.log.likelihood0

Log-likelihood of the mixture model

Description

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

Usage

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

Arguments

x_data The observed data

w Vector of mixture 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)

```
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 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)

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)
```

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)

overfittingMFA 35

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: $\beta=1$.

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

gibbs_z Optional

Value

List of files

Author(s)

overfittingMFA_CCC Basic MCMC sampler for CCC

Description

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

Usage

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

Arguments

x_data normalized data

originalX observed raw data (only for plotting purpose)

outputDirectory

Name of the output folder

Kmax Number of mixture components

m Number of iterationsthinning Thinning of chainburn Burn-in period

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

alpha_prior Parameters of the Dirichlet prior distribution of mixture weights.

alpha_sigma Prior parameter 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)

overfittingMFA_CCU 37

overfittingMFA_CCU I

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

Value

List of files

Author(s)

overfittingMFA_CUC Bas

Basic MCMC sampler for CUC

Description

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

Usage

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

Arguments

x_data normalized data

originalX observed raw data (only for plotting purpose)

outputDirectory

Name of the output folder

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_CUU 39

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)

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

Author(s)

overfittingMFA_Sj 41

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: $\beta=1$.

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

gibbs_z Optional

Value

List of files

overfittingMFA_UCC 43

Author(s)

Panagiotis Papastamoulis

overfittingMFA_UCC

Basic MCMC sampler for CCC

Description

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

Usage

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

Arguments

x_data normalized data

originalX observed raw data (only for plotting purpose)

outputDirectory

Name of the output folder

Kmax Number of mixture components

m Number of iterationsthinning Thinning of chainburn Burn-in period

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

alpha_prior Parameters of the Dirichlet prior distribution of mixture weights.

alpha_sigma Prior parameter 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_UUC

Basic MCMC sampler for UUC

Description

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

Usage

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

Arguments

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)

overfitting_q0 45

overfitting_q0	MCMC sampler for $q = 0$	

Description

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

Usage

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

Arguments

x_data normalized data

originalX observed raw data (only for plotting purpose)

outputDirectory

Name of the output folder

Kmax Number of mixture components

m Number of iterationsthinning Thinning of chainburnBurn-in period

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

alpha_prior Parameters of the Dirichlet prior distribution of mixture weights.

alpha_sigma Prior parameter 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)

```
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)

plot.fabMix.object 47

Description

This function plots fabMix function.

Usage

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

Arguments

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

what One of the "BIC", "classification_matplot", "classification_pairs", "correlation",

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

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

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

... ignored.

Details

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

Author(s)

Panagiotis Papastamoulis

References

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

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

48 readLambdaValues

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.
... ignored.
```

Details

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

Author(s)

Panagiotis Papastamoulis

	D 17 11 1
readLambdaValues	Read Lambda values.

Description

Function to read Lambda values from file.

Usage

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

Arguments

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

simData 49

Value

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

Author(s)

Panagiotis Papastamoulis

simData	Synthetic data generator	

Description

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

Usage

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

Arguments

sameSigma	Logical.
sameLambda	Logical.
p	The dimension of the multivariate normal distribution $(p > 1)$.
q	Number of factors. It should be strictly smaller than p.
K.true	The number of mixture components (clusters).
n	Sample size.
loading_means	A vector which contains the means of blocks of factor loadings. Default: loading_means = $c(-30, -20, -10, 10, 20, 30)$.
loading_sd	A vector which contains the standard deviations of blocks of factor loadings. Default: loading_sd <- rep(2, length(loading_means)).
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 $k = 1, \dots, K$; $r = 1, \dots, p$; $j = 1, \dots, q$.

50 update_all_y

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

 $1,\ldots,p$.

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

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

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

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

Note

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

Author(s)

Panagiotis Papastamoulis

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 51

update_all_y_Sj

Gibbs sampling for y

Description

Gibbs sampling for \boldsymbol{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

Lambda	Factor	loadings
--------	--------	----------

K Number of components

g Prior parameterh Prior parameter

Value

 Ω^{-1}

Author(s)

Panagiotis Papastamoulis

update_OmegaINV_Cxx

Gibbs sampling for Ω^-1 for Cxx model

Description

Gibbs sampling for Ω^{-1} for Cxx model

Usage

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

Arguments

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

Value

 Ω^{-1}

Author(s)

```
update_SigmaINV_faster
```

Gibbs sampling for Σ^-1

Description

Gibbs sampling for Σ^{-1}

Usage

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

Arguments

x_da	ta	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)

Panagiotis Papastamoulis

```
update_SigmaINV_faster_q0
```

Gibbs sampling for Σ^-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
```

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

```
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)

Panagiotis Papastamoulis

update_SigmaINV_xCC

Gibbs sampling for Σ^-1 for xCC models

Description

Gibbs sampling for Σ^{-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

 Σ^{-1}

Author(s)

Panagiotis Papastamoulis

update_SigmaINV_xUC Gi

Gibbs sampling for Σ^-1 per component for xUC models

Description

Gibbs sampling for Σ^{-1} per component for xUC models

Usage

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

Arguments

x_data Data

z Allocation vector

y Factors

Lambda Factor loadings mu Marginal means

K Number of components

alpha_sigma Prior parameter beta_sigma Prior parameter

Value

 Σ^{-1}

update_z2 57

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)

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)
```

58 update_z4

Arguments

w Mixture weightsmu Marginal meansLambda Factor loadings

SigmaINV Precision matrix per component

K Number of components

x_data Data

Value

Allocation vector

Author(s)

Panagiotis Papastamoulis

update_z4 $Collapsed\ Gibbs\ for\ z$

Description

Collapsed Gibbs for z

Usage

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

Arguments

w Mixture weightsmu Marginal meansLambda Factor loadingsSigmaINV Precision matrix

K Number of components

x_data Data

Value

Allocation vector

Author(s)

update_z4_Sj 59

update_z4_Sj

Collapsed Gibbs for z

Description

Collapsed Gibbs for z

Usage

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

Arguments

w Mixture weightsmu Marginal meansLambda Factor loadings

SigmaINV Precision matrix per component

K Number of components

x_data Data

Value

Allocation vector

Author(s)

Panagiotis Papastamoulis

update_z_b

Gibbs sampling for z

Description

Gibbs sampling for z

Usage

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

60 update_z_b_Sj

Arguments

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

K Number of components

x_data Data

Value

Allocation vector

Author(s)

Panagiotis Papastamoulis

update_z_b_Sj

Gibbs sampling for z

Description

Gibbs sampling for z

Usage

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

Arguments

w Mixture weightsmu Marginal meansLambda Factor loadingsy Matrix of factors

SigmaINV Precision matrix per component

K Number of components

x_data Data

Value

Allocation vector

Author(s)

 $update_z_q0$ 61

update_z_q0

Gibbs sampling for z for q = 0

Description

Gibbs sampling for z

Usage

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

Arguments

w Mixture weightsmu Marginal means

SigmaINV Precision matrix per component

K Number of components

x_data Data

Value

Allocation vector

Author(s)

Panagiotis Papastamoulis

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

Description

Gibbs sampling for z

Usage

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

Arguments

w Mixture weights mu Marginal means

SigmaINV Precision matrix per component

K Number of components

x_data Data

62 waveDataset1500

Value

Allocation vector

Author(s)

Panagiotis Papastamoulis

waveDataset1500

Wave dataset

Description

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

Usage

waveDataset1500

Format

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

Source

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

References

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

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

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