Package 'fabMix'

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Title Overfitting Bayesian Mixtures of Factor Analyzers with an
Unknown Number of Components
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Description
Model-based clustering of multivariate continuous data with or without missing values. The un-
derlying model is a Bayesian mixture of factor analyzers with a large number of compo-
nents (overfitting mixture). Suitable prior assumptions ensure that asymptotically the extra com-
ponents will have zero posterior weight (empty), therefore, the inference on the number of clus-
ters is based on the "alive" components. The number of factors is considered fixed, and the opti-

ing are dealt by post-processing the simulated output with the ECR algorithm.

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Imports MASS, doParallel, foreach, label.switching, mvtnorm, doRNG

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R topics documented:

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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)

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.

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)
## 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)
```

 ${\tt complete.log.likelihood}$

Complete log-likelihood function

Description

Complete log-likelihood function

Usage

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

Arguments

		_
Х	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)

```
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_Sj
```

Complete log-likelihood function

Description

Complete log-likelihood function

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

Arguments

x_data Data

w Mixture weightsmu Marginal meansLambda Factor loadings

SigmaINV Precision matrix (inverse covariance) per component
z Allocation vector of the data to the mixture components

Value

complete log-likelihood value

Author(s)

Panagiotis Papastamoulis

Description

This function simulates 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

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

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 .

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

```
{\tt compute\_sufficient\_statistics}
```

Compute sufficient statistics

Description

Compute sufficient statistics given y and z.

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

Arguments

У	Matrix of factors
Z	Allocation vector

K Number of components

x_data Data

Value

A list with six entries of sufficient statistics.

Author(s)

Panagiotis Papastamoulis

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.

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 of the package	

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)
```

Arguments

sameSigma	Logical value denoting the parameterization of the error variance per component. If TRUE, the parameterization $\Sigma_1 = \ldots = \Sigma_K$ is fitted.
dirPriorAlphas	The prior Dirichlet parameters for each chain.
rawData	The observed data as an $n \times p$ matrix. Clustering is performed on the rows of the matrix.
outDir	Name of the output folder.
Kmax	Number of components in the overfitted mixture. Default: 20.
mCycles	Number of MCMC cycles. Each cycle consists of nIterPerCycle MCMC iterations. At the end of each cycle a swap of the state of two randomly chosen adjacent chains is attempted.
burnCycles	Number of cycles that will be discarded as burn-in period.
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.
gibbs_z	Select the gibbs sampling scheme for updating latent allocations of mixture model. Default value: 1.

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

References

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

See Also

dealWithLabelSwitching

Examples

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

```
compute_regularized_expression = TRUE, Km = Kmax)
## End(Not run)
```

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

```
fab \verb|Mix_missing_values| (same Sigma, dir Prior Alphas, raw Data, out Dir, \verb|Kmax, mCycles|) (same Sigma, dir Prior Alphas, raw Data, out Dir, \verb|Kmax, mCycles|) (same Sigma, dir Prior Alphas, raw Data, out Dir, \verb|Kmax, mCycles|) (same Sigma, dir Prior Alphas, raw Data, out Dir, \verb|Kmax, mCycles|) (same Sigma, dir Prior Alphas, raw Data, out Dir, \verb|Kmax, mCycles|) (same Sigma, dir Prior Alphas, raw Data, out Dir, \verb|Kmax, mCycles|) (same Sigma, dir Prior Alphas, raw Data, out Dir, \verb|Kmax, mCycles|) (same Sigma, dir Prior Alphas, raw Data, out Dir, \verb|Kmax, mCycles|) (same Sigma, dir Prior Alphas, raw Data, out Dir, \verb|Kmax, mCycles|) (same Sigma, dir Prior Alphas, raw Data, out Dir, \verb|Kmax, mCycles|) (same Sigma, dir Prior Alphas, raw Data, out Dir, \verb|Kmax, mCycles|) (same Sigma, dir Prior Alphas, raw Data, out Dir, make Data, out Dir, 
burnCycles, g, h, alpha_sigma, beta_sigma, q, normalize,
 thinning, zStart, nIterPerCycle, gibbs_z)
```

Arguments

sameSigma	Logical value denoting the parameterization of the error variance per component. If TRUE, the parameterization $\Sigma_1 = \ldots = \Sigma_K$ is fitted.
dirPriorAlphas	The prior Dirichlet parameters for each chain.
rawData	The observed data as an $n \times p$ matrix. Clustering is performed on the rows of the matrix.
outDir	Name of the output folder.
Kmax	Number of components in the overfitted mixture. Default: 20.
mCycles	Number of MCMC cycles. Each cycle consists of nIterPerCycle MCMC iterations. At the end of each cycle a swap of the state of two randomly chosen adjacent chains is attempted.
burnCycles	Number of cycles that will be discarded as burn-in period.
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.
gibbs_z	Select the gibbs sampling scheme for updating latent allocations of mixture model. Default value: 1.

Value

List of files written to outDir

Note

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

Author(s)

Panagiotis Papastamoulis

References

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

See Also

dealWithLabelSwitching

Examples

```
## Not run:
# simulate a synthetic dataset along the lines of the paper:
n = 1000
                     # sample size
p = 40
                     # number of variables
q = 4
                     # number of factors
                     # number of clusters
K = 10
sINV_diag = 1/((1:p)) # diagonal of inverse variance of errors
syntheticDataset <- simData(K.true = K, n = n, q = q, p = p, sINV_values = sINV_diag)
# define parameters
Kmax <- 20 # number of overfitted mixture components
nChains <- 8 # number of parallel chains
dN < -1
# Dirichlet prior of mixture weights per chain.
    The target chain corresponds to the first entry.
dirPriorAlphas <- c(1, 1 + dN * (2:nChains - 1))/Kmax
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)
```

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

Details

If necessary, more details than the description above

applied only for the DIC computation.

Value

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

myDirichlet

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_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.

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

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Arguments

x_dataw 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

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: $\beta=1$.

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)

output Directory

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.

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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_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

 $\begin{array}{ll} {\rm g} & {\rm Prior\ parameter}\ g.\ {\rm Default\ value:}\ g=2. \\ {\rm h} & {\rm Prior\ parameter}\ h.\ {\rm Default\ value:}\ h=1. \end{array}$

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_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. overfitting_q0 23

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

 $\label{eq:mcmc} \textit{overfitting_q0} \qquad \qquad \textit{MCMC sampler for } q = 0$

Description

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

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: $\alpha = 2$.

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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

simData	Synthetic data generator	

Description

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

Usage

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

Arguments

sameSigma	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).

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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 μ_{kr} , k = 1, ..., 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.

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

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Author(s)

Panagiotis Papastamoulis

update_all_y_Sj

Gibbs sampling for y

Description

Gibbs sampling for y

Usage

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

Arguments

x_data Data

mu Marginal means

SigmaINV Precision matrix per component

Lambda Factor loadings
z Allocation vector

Value

A matrix with generated factors

Author(s)

Panagiotis Papastamoulis

update_OmegaINV

Gibbs sampling for Ω^-1

Description

Gibbs sampling for Ω^{-1}

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

Arguments

K Number of components

g Prior parameterh Prior parameter

Value

 Ω^{-1}

Author(s)

Panagiotis Papastamoulis

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_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 vectormu 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 {\it Gibbs\ sampling\ for\ } \Sigma^{^{-}}-1\ per\ component
```

Description

Gibbs sampling for Σ^{-1} per component

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

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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_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)

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update_z2_Sj

Collapsed Gibbs for z using matrix inversion lemma

Description

Collapsed Gibbs for z using matrix inversion lemma

Usage

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

Arguments

w Mixture weightsmu Marginal meansLambda Factor loadings

SigmaINV Precision matrix per component

K Number of components

x_data Data

Value

Allocation vector

Author(s)

Panagiotis Papastamoulis

update_z4

Collapsed Gibbs for z

Description

Collapsed Gibbs for z

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

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Arguments

w Mixture weightsmu Marginal meansLambda Factor loadingsSigmaINV Precision matrix

K Number of components

x_data Data

Value

Allocation vector

Author(s)

Panagiotis Papastamoulis

update_z4_Sj $Collapsed\ Gibbs\ for\ z$

Description

Collapsed Gibbs for z

Usage

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

Arguments

w Mixture weightsmu Marginal meansLambda Factor loadings

SigmaINV Precision matrix per component

K Number of components

x_data Data

Value

Allocation vector

Author(s)

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update_z_b

Gibbs sampling for z

Description

Gibbs sampling for z

Usage

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

Arguments

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

K Number of components

x_data Data

Value

Allocation vector

Author(s)

Panagiotis Papastamoulis

update_z_b_Sj

Gibbs sampling for z

Description

Gibbs sampling for z

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

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Arguments

w Mixture weightsmu Marginal meansLambda Factor loadingsy Matrix of factors

SigmaINV Precision matrix per component

K Number of components

x_data Data

Value

Allocation vector

Author(s)

Panagiotis Papastamoulis

update_z_q0

Gibbs sampling for z for q = 0

Description

Gibbs sampling for z

Usage

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

Arguments

w Mixture weightsmu Marginal means

SigmaINV Precision matrix per component

K Number of components

x_data Data

Value

Allocation vector

Author(s)

34 waveDataset1500

waveDataset1500

Wave dataset

Description

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

Usage

waveDataset1500

Format

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

Source

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

References

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

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

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