

Package ‘fabMix’

January 26, 2017

Type Package

Title Overfitting Bayesian Mixtures of Factor Analyzers with an
Unknown Number of Components

Version 1.0

Date 2017-01-25

Author Panagiotis Papastamoulis

Maintainer Panagiotis Papastamoulis <papapast@yahoo.gr>

Description

Model-based clustering of multivariate continuous data with possibly complex covariance structure. The underlying model is a Bayesian mixture of factor analyzers with a large number of components (overfitting mixture). Suitable prior assumptions ensure that asymptotically the extra components will have zero posterior weight (empty), therefore, the inference on the number of clusters is based on the “alive” components. The number of factors is considered fixed, and the optimal one can be estimated using information criteria. Identifiability issues related to label switching are dealt by post-processing the simulated output with the ECR algorithm.

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

License GPL-2

NeedsCompilation no

R topics documented:

fabMix-package	2
complete.log.likelihood	3
compute_A_B_G_D_and_simulate_mu_Lambda	4
compute_sufficient_statistics	4
dealWithLabelSwitching_same_sigma	5
fabMix	6
getStuffForDIC	7
log_dirichlet_pdf	8
myDirichlet	9
observed.log.likelihood0	9
overfittingMFA	10
update_all_y	11

update_OmegaINV	11
update_SigmaINV_faster	12
update_z4	13
update_z_b	13

Index	15
--------------	-----------

fabMix-package	<i>Overfitting Bayesian Mixtures of Factor Analyzers with an Unknown Number of Components</i>
----------------	---

Description

Model-based clustering of multivariate continuous data with possibly complex covariance structure. 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.

Details

Model-based clustering of multivariate continuous data with possibly complex covariance structure. 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>

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_same_sigma](#), [getStuffForDIC](#)

Examples

```
runif(1)
```

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 weights
mu	Marginal means
Lambda	Factor loadings
SigmaINV	Precision matrix (inverse covariance)
z	Allocation vector of the data to the mixture components

Value

complete log-likelihood value

Author(s)

Panagiotis Papastamoulis

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	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)

Panagiotis Papastamoulis

dealWithLabelSwitching_same_sigma

Apply label switching algorithms for the Σ model

Description

This functions is a wrapper for the `label.switching` package and applies the ECR and ECR.ITERATIVE.1 algorithms. The model should have the same variance of error terms per cluster.

Usage

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

Arguments

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

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(dirPriorAlphas, rawData, outDir, Kmax, mCycles, burnCycles,
g, h, alpha_sigma, beta_sigma, q, normalize, thinning, zStart, nIterPerCycle)
```

Arguments

<code>dirPriorAlphas</code>	The prior Dirichlet parameters for each chain.
<code>rawData</code>	The observed data as an $n \times p$ matrix. Clustering is performed on the rows of the matrix.
<code>outDir</code>	Name of the output folder.
<code>Kmax</code>	Number of components in the overfitted mixture. Default: 20.
<code>mCycles</code>	Number of MCMC cycles. Each cycle consists of <code>nIterPerCycle</code> MCMC iterations. At the end of each cycle a swap of the state of two randomly chosen adjacent chains is attempted.
<code>burnCycles</code>	Number of cycles that will be discarded as burn-in period.
<code>g</code>	Prior parameter g . Default value: $g = 2$.
<code>h</code>	Prior parameter h . Default value: $h = 1$.
<code>alpha_sigma</code>	Prior parameter α . Default value: $\alpha = 2$.
<code>beta_sigma</code>	Prior parameter β . Default value: $\beta = 1$.
<code>q</code>	Number of factors q , where $1 \leq q \leq L$. An error is thrown if the Ledermann bound (L) is exceeded.
<code>normalize</code>	Should the observed data be normalized? Default value: TRUE.
<code>thinning</code>	Optional integer denoting the thinning of the kept MCMC cycles.
<code>zStart</code>	Optional starting value for the allocation vector.
<code>nIterPerCycle</code>	Number of iteration per MCMC cycle. Default value: 10.

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_same_sigma` 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_same_sigma](#)

getStuffForDIC

Compute information criteria

Description

This function computes four information criteria for a given run of the `fabMix` algorithm, namely: AIC, BIC, DIC and DIC_2 . Given various runs with different number of factors, the selected model corresponds to the one with the smallest value of the selected criterion.

Usage

```
getStuffForDIC(x_data, outputFolder, q, burn, Km, normalize, discardLower)
```

Arguments

<code>x_data</code>	Observed data.
<code>outputFolder</code>	Name of the folder where the <code>fabMix</code> function has saved its output.
<code>q</code>	Number of factors. Note that this should coincide with the number of factors in the <code>fabMix</code> run.
<code>burn</code>	Discard observations as burn-in period (optional).
<code>Km</code>	Number of components in the overfitted mixture model. Note that this should coincide with the same entry in the <code>fabMix</code> 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.

Note

It is well known that DIC tends to overfit, so it is advised to compare models with different number of factors using AIC or BIC.

Author(s)

Panagiotis Papastamoulis

log_dirichlet_pdf	<i>Log-density function of the Dirichlet distribution</i>
-------------------	---

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 $D(\alpha_1, \dots, \alpha_k)$ evaluated at w_1, \dots, w_k .

Author(s)

Panagiotis Papastamoulis

myDirichlet	<i>Simulate from the Dirichlet distribution</i>
-------------	---

Description

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

Usage

```
myDirichlet(alpha)
```

Arguments

alpha	Parameter vector
-------	------------------

Value

Simulated vector

Author(s)

Panagiotis Papastamoulis

observed.log.likelihood0	<i>Log-likelihood of the mixture model</i>
--------------------------	--

Description

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

Usage

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

Arguments

x_data	The observed data
w	Vector of mixture weights
mu	Vector of marginal means
Lambda	Factor loadings
Sigma	Common covariance matrix of the errors per cluster
z	Allocation vector

Value

Log-likelihood value

Author(s)

Panagiotis Papastamoulis

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 iterations
thinning	Thinning of chain
burn	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

update_all_y	<i>Gibbs sampling for y</i>
--------------	--

Description

Gibbs sampling for y

Usage

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

Arguments

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

Value

A matrix with generated factors

Author(s)

Panagiotis Papastamoulis

update_OmegaINV	<i>Gibbs sampling for Ω^{-1}</i>
-----------------	--

Description

Gibbs sampling for Ω^{-1}

Usage

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

Arguments

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

Value

Ω^{-1}

Author(s)

Panagiotis Papastamoulis

update_SigmaINV_faster	<i>Gibbs sampling for $\Sigma^{\wedge}-1$</i>
------------------------	--

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)

Panagiotis Papastamoulis

update_z4	<i>Collapsed Gibbs for z</i>
-----------	---

Description

Collapsed Gibbs for z

Usage

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

Arguments

w	Mixture weights
mu	Marginal means
Lambda	Factor loadings
SigmaINV	Precision matrix
K	Number of components
x_data	Data

Value

Allocation vector

Author(s)

Panagiotis Papastamoulis

update_z_b	<i>Gibbs sampling for z</i>
------------	--

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

Index

*Topic **package**

- fabMix-package, [2](#)
- complete.log.likelihood, [3](#)
- compute_A_B_G_D_and_simulate_mu_Lambda,
[4](#)
- compute_sufficient_statistics, [4](#)
- dealWithLabelSwitching_same_sigma, [3](#), [5](#),
[7](#)
- fabMix, [3](#), [6](#)
- fabMix-package, [2](#)
- getStuffForDIC, [3](#), [7](#)
- log_dirichlet_pdf, [8](#)
- myDirichlet, [9](#)
- observed.log.likelihood0, [9](#)
- overfittingMFA, [10](#)
- update_all_y, [11](#)
- update_OmegaINV, [11](#)
- update_SigmaINV_faster, [12](#)
- update_z4, [13](#)
- update_z_b, [13](#)