Package 'BayesBinMix'

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Type Package

Title Bayesian Estimation of Mixtures of Multivariate Bernoulli Distributions

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Description Fully Bayesian inference for estimating the number of clusters and related parameters to heterogeneous binary data.

Imports label.switching, foreach, doParallel

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R topics documented:

`BayesBinMix-package` *Bayesian Estimation of Mixtures of Multivariate Bernoulli Distributions*

Description

Fully Bayesian inference for estimating the number of clusters and related parameters to heterogeneous binary data.

Details

This package can be used in order to cluster multivariate binary data. The main function of the package is `coupledMetropolis`.

The input is an $n \times d$ binary array where n and d denote the number of observations and dimension of the data. The underlying model is a mixture of independent multivariate Bernoulli distributions with an unknown number of components:

$$x_i \sim \sum_{k=1}^{K} \pi_k \prod_{j=1}^{d} f(x_{ij}; \theta_{kj}),$$

with $x_i = (x_{i1}, \ldots, x_{id})$; $d > 1$, independent for $i = 1, \ldots, n$. The term $f(x_{ij}; \theta_{kj})$ denotes the probability density function of the Bernoulli distribution with parameter $\theta_{kj} \in (0, 1)$. The number of clusters K is a random variable with support $\{1, \ldots, K_{\text{max}}\}$, where K_{max} is an upper bound for the number of clusters. The model uses the following prior assumptions:

$$K \sim \text{discrete}\{1, \ldots, K_{\text{max}}\}$$

$$(\pi_1, \ldots, \pi_K)|K \sim \text{Dirichlet}(\gamma, \ldots, \gamma)$$

$$\theta_{kj}|K \sim \text{Beta}(\alpha, \beta); \quad \text{independent for} \quad k = 1, \ldots, K; j = 1, \ldots, d.$$

The discrete distribution on the number of clusters it can be a truncated Poisson(1) or Uniform distribution. The model uses data augmentation by also considering the (latent) allocation variable z_i, which a priori assigns observation i to cluster $k = 1, \ldots, K$ with probability $P(z_i = k|K, \pi_1, \ldots, \pi_K) = \pi_k$ independently for $i = 1, \ldots, n$.

In order to infer the parameters of the model, a Markov chain Monte Carlo (MCMC) approach is adopted. Given K, the component-specific parameters π_k and θ_{kj} are integrated out and a collapsed allocation sampler which also updates the number of clusters (Nobile and Fearnside, 2007) is implemented. In order to improve the mixing of the simulated chain, a Metropolis-coupled MCMC sampler (Altekar et al., 2004) is incorporated. In particular, various heated chains are run in parallel and swaps are proposed between pairs of chains. The number of chains should be equal to the number of available cores. Each chain runs in parallel using the packages `foreach` and `doParallel`.

After inferring the most probable number of clusters, the simulated parameters which correspond to the specific number of components are post-processed in order to undo the label switching problem. For this purpose the `label.switching` (Papastamoulis, 2016) package is used.

Author(s)

Panagiotis Papastamoulis

Maintainer: Panagiotis Papastamoulis

References

Altekar G, Dwarkadas S, Huelsenbeck JP, Ronquist F. (2004): Parallel Metropolis coupled Markov chain Monte Carlo for Bayesian phylogenetic inference. Bioinformatics 20(3): 407-415.

Nobile A and Fearnside A (2007): Bayesian finite mixtures with an unknown number of components: The allocation sampler. Statistics and Computing, 17(2): 147-162.

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.

See Also

coupledMetropolis

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allocationSamplerBinMix

The allocation sampler algorithm.

Description

This function implements the collapsed allocation sampler of Nobile and Fearnside (2007) at the context of mixtures of multivariate Bernoulli distributions.

Usage

```
allocationSamplerBinMix(Kmax, alpha, beta, gamma, m, burn, data,
thinning, z.true, ClusterPrior, ejectionAlpha, Kstart, outputDir,
metropolisMoves, reorderModels, heat, zStart, LS)
```

Arguments

Kmax	Maximum number of clusters (integer, at least equal to two).
alpha	First shape parameter of the Beta prior distribution (strictly positive). Defaults to 1.
beta	Second shape parameter of the Beta prior distribution (strictly positive). Defaults to 1.
gamma	Kmax-dimensional vector (positive) corresponding to the parameters of the Dirichlet prior of the mixture weights. Default value: rep(1,Kmax).
m	Number of MCMC iterations.
burn	The number of initial MCMC iterations that will be discarded as burn-in period.
data	Binary data array.

`thinning`	Integer that defines a thinning of the reported MCMC sample. Under the default setting, every 5th MCMC iteration is saved.
`z.true`	An optional vector of cluster assignments considered as the ground-truth clustering of the observations. Useful for simulations.
`ClusterPrior`	Character string specifying the prior distribution of the number of clusters on the set $\{1, \ldots, K_{max}\}$. Available options: `poisson` or `uniform`. It defaults to the truncated Poisson distribution.
`ejectionAlpha`	Probability of ejecting an empty component. Defaults to 0.2.
`Kstart`	Initial value for the number of clusters. Defaults to 1.
`outputDir`	The name of the produced output folder.
`metropolisMoves`	A vector of character strings with possible values `M1`, `M2`, `M3`, `M4`. Each entry specifies Metropolis-Hastings type moves on the latent allocation variables.
`reorderModels`	Character string specifying whether to post-process the MCMC sample of each distinct generated value of `K`. The default setting is `onlyMAP` and in this case only the part of the MCMC sample that corresponds to the most probable number of clusters is reordered.
`heat`	The temperature of the simulated chain, that is, a scalar in the set $(0, 1]$.
`zStart`	n-dimensional integer vector of latent allocations to initialize the sampler.
`LS`	Boolean indicating whether to post-process the MCMC sample using the label switching algorithms.

Details

The output is reordered according to the following label-switching solving algorithms: ECR, ECR-ITERATIVE-1 and STEPHENS. In most cases the results of these different algorithms are identical.

Note

This function is recursively called inside the `coupledMetropolis` function.

Author(s)

Panagiotis Papastamoulis

References

Nobile A and Fearnside A (2007): Bayesian finite mixtures with an unknown number of components: The allocation sampler. Statistics and Computing, 17(2): 147-162.

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.

See Also

`coupledMetropolis`

collapsedGibbsBinMix *collapsed Gibbs sampler*

Description

This function applied collapsed Gibbs sampling assuming that the number of mixture components is known.

Usage

```
collapsedGibbsBinMix(alpha, beta, gamma, K, m, burn, data, thinning, z.true, outputDir)
```

Arguments

alpha	First shape parameter of the Beta prior distribution (strictly positive). Defaults to 1.
beta	Second shape parameter of the Beta prior distribution (strictly positive). Defaults to 1.
gamma	K-dimensional vector (positive) corresponding to the parameters of the Dirichlet prior of the mixture weights. Default value: `rep(1,K)`.
K	Number of clusters.
m	Number of MCMC iterations.
burn	The number of initial MCMC iterations that will be discarded as burn-in period.
data	Binary data array.
thinning	Integer that defines a thinning of the reported MCMC sample. Under the default setting, every 5th MCMC iteration is saved.
z.true	An optional vector of cluster assignments considered as the ground-truth clustering of the observations. Useful for simulations.
outputDir	The name of the produced output folder.

Note

Not really used.

Author(s)

Panagiotis Papastamoulis

complete.loglikelihood *complete log-likelihood*

Description

Returns the complete log-likelihood of the mixture.

Usage

```
complete.loglikelihood(x, z, pars)
```

Arguments

x	Binary data.
z	Latent allocations vector.
pars	Parameters of the mixture.

Value

Complete log-likelihood value.

Author(s)

Panagiotis Papastamoulis

coupledMetropolis *Metropolis-coupled Markov chain Monte Carlo sampler*

Description

Main function of the package. The algorithm consists of the allocation sampler combined with a MC3 scheme.

Usage

```
coupledMetropolis(Kmax, nChains, heats, binaryData, outPrefix, ClusterPrior,
 m, alpha, beta, gamma, z.true, ejectionAlpha)
```

Arguments

`Kmax`	Maximum number of clusters (integer, at least equal to two).
`nChains`	Number of parallel (heated) chains. Ideally, it should be equal to the number of available threads.
`heats`	`nChains`-dimensional vector specifying the temperature of each chain: the 1st entry should always be equal to 1 and the rest of them lie on the set: $(0, 1]$.
`binaryData`	The observed binary data (array).
`outPrefix`	The name of the produced output folder. An error is thrown if the directory exists.
`ClusterPrior`	Character string specifying the prior distribution of the number of clusters on the set $\{1, \ldots, K_{max}\}$. Available options: `poisson` or `uniform`. It defaults to the truncated Poisson distribution.
`m`	The number of MCMC cycles. At the end of each cycle a swap between a pair of heated chains is attempted. Each cycle consists of 10 iterations.
`alpha`	First shape parameter of the Beta prior distribution (strictly positive). Defaults to 1.
`beta`	Second shape parameter of the Beta prior distribution (strictly positive). Defaults to 1.
`gamma`	`Kmax`-dimensional vector (positive) corresponding to the parameters of the Dirichlet prior of the mixture weights. Default value: `rep(1,Kmax)`.
`z.true`	An optional vector of cluster assignments considered as the ground-truth clustering of the observations. Useful for simulations.
`ejectionAlpha`	Probability of ejecting an empty component. Defaults to 0.2.

Details

In the case that the most probable number of clusters is larger than 1, the output is post-processed using the label.switching package.

Value

The final output is written to the directory `outPrefix`. It consists of the following files:

`K.allChains.txt`
: `m`$\times$`nChains` matrix containing the simulated values of the number of clusters (K) per chain.

`K.txt`
: the `m` simulated values of the number of clusters (K) of the cold chain (posterior distribution).

`p.varK.txt`
: the simulated values of the mixture weights (not identifiable).

`rawMCMC.mapK.KVALUE.txt`
: the raw MCMC output which corresponds to the most probable model (not identifiable).

`reorderedMCMC-ECR-ITERATIVE1.mapK.KVALUE.txt`
: the reordered MCMC output which corresponds to the most probable model, reordered according to the `ECR-ITERATIVE-1` algorithm.

`reorderedMCMC-ECR.mapK.KVALUE.txt`
: the reordered MCMC output which corresponds to the most probable model, reordered according to the `ECR` algorithm.

`reorderedMCMC-STEPHENS.mapK.KVALUE.txt`
: the reordered MCMC output which corresponds to the most probable model, reordered according to the `STEPHENS` algorithm.

`reorderedSingleBestClusterings.mapK.KVALUE.txt`
: the most probable allocation of each observation after reordering the MCMC sample which corresponds to the most probable number of clusters.

`theta.varK.txt`
: the simulated values of Bernoulli parameters (not identifiable).

`z-ECR-ITERATIVE1.mapK.KVALUE.txt`
: the reordered simulated latent allocations which corresponds to the most probable model, reordered according to the `ECR-ITERATIVE-1` algorithm.

`z-ECR.mapK.KVALUE.txt`
: the reordered simulated latent allocations which corresponds to the most probable model, reordered according to the `ECR` algorithm.

`z-KL.mapK.KVALUE.txt`
: the reordered simulated latent allocations which corresponds to the most probable model, reordered according to the `STEPHENS` algorithm.

`z.varK.txt`
: the simulated latent allocations (not identifiable).

`classificationProbabilities.mapK.KVALUE.csv`
: the reordered classification probabilities per observation after reordering the most probable number of clusters with the `ECR` algorithm.

`KVALUE` will be equal to the inferred number of clusters. Note that the label switching part is omitted in case that the most probable number of clusters is equal to 1.

Author(s)

Panagiotis Papastamoulis

References

Altekar G, Dwarkadas S, Huelsenbeck JP, Ronquist F. (2004): Parallel Metropolis coupled Markov chain Monte Carlo for Bayesian phylogenetic inference. Bioinformatics 20(3): 407-415.

Nobile A and Fearnside A (2007): Bayesian finite mixtures with an unknown number of components: The allocation sampler. Statistics and Computing, 17(2): 147-162.

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.

Examples

```
#generate dataset from a mixture of 2 ten-dimensional Bernoulli distributions.
set.seed(1)
d <- 10 # number of columns
n <- 50 # number of rows (sample size)
K <- 2   # true number of clusters
p.true <- myDirichlet(rep(10,K)) # true weight of each cluster
```

```
z.true <- numeric(n) # true cluster membership
z.true <- sample(K,n,replace=TRUE,prob = p.true)
theta.true <- array(data = NA, dim = c(K,d)) #true probability of positive responses per cluster
for(j in 1:d){
    theta.true[,j] <- rbeta(K, shape1 = 1, shape2 = 1)
}
x <- array(data=NA,dim = c(n,d)) # data: n X d array
for(k in 1:K){
        myIndex <- which(z.true == k)
        for (j in 1:d){
             x[myIndex,j] <- rbinom(n = length(myIndex), size = 1, prob = theta.true[k,j])
        }
}
# number of heated paralled chains
nChains <- 2
heats <- seq(1,0.8,length = nChains)
# NOTE: only m = 5 iterations are used here (modify to m = 1000 for non-erroneous results)
coupledMetropolis(Kmax = 10,nChains = nChains,heats =  heats,binaryData = x,
outPrefix = BayesBinMixExample,ClusterPrior = poisson,m = 5)
# it is also advised to use z.true = z.true in order to directly compare with the true values.
# in general it is advised to use at least 4 chains with heats <- seq(1,0.3,length = nChains)
```

`dealWithLabelSwitching` *Label switching algorithms*

Description

This is a wrapper for the `label.switching` package. It is used to post-process the generated MCMC sample in order to undo the label switching problem. This function is called internally to the `coupledMetropolis` command.

Usage

```
dealWithLabelSwitching(outDir, reorderModels, binaryData, z.true)
```

Arguments

`outDir`	The directory where the output of `coupledMetropolis` was previously produced.
`reorderModels`	Boolean value indicating whether to reorder the MCMC corresponding to each distinct generated value of number of clusters or not.
`binaryData`	The input data.
`z.true`	An optional vector of cluster assignments considered as the ground-truth clustering of the observations. Useful for simulations.

Details

See the `label.switching` package.

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.

`gibbsBinMix` *Standard Gibbs sampler*

Description

This function implements full Gibbs sampling to simulate an MCMC sample from the posterior distribution assuming known number of mixture components.

Usage

```
gibbsBinMix(alpha, beta, gamma, K, m, burn, data, thinning, z.true, outputDir)
```

Arguments

`alpha`	First shape parameter of the Beta prior distribution (strictly positive). Defaults to 1.
`beta`	Second shape parameter of the Beta prior distribution (strictly positive). Defaults to 1.
`gamma`	`Kmax`-dimensional vector (positive) corresponding to the parameters of the Dirichlet prior of the mixture weights. Default value: `rep(1,Kmax)`.
`K`	Number of clusters.
`m`	Number of MCMC iterations.
`burn`	Burn-in period.
`data`	Binary data.
`thinning`	Thinning of the simulated chain.
`z.true`	An optional vector of cluster assignments considered as the ground-truth clustering of the observations. Useful for simulations.
`outputDir`	Output directory.

Details

Not really used.

Author(s)

Panagiotis Papastamoulis

`myDirichlet` *Simulate from Dirichlet distribution*

Description

This function simulates random vectors from a Dirichlet distribution.

Usage

```
myDirichlet(alpha)
```

Arguments

`alpha`	Vector of positive numbers denoting the parameters of the Dirichlet distribution.

Author(s)

Panagiotis Papastamoulis

`toSolve` *An equation to solve*

Description

Approximately solve the equation (25) of Nobile and Fearnside (2007).

Usage

```
toSolve(a, n, p0)
```

Arguments

`a`	Positive number.
`n`	Positive integer.
`p0`	Probability.

Author(s)

Panagiotis Papastamoulis

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