Package 'bayMDS'

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Type Package

Title Bayesian Multidimensional Scaling and Choice of Dimension

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Description Bayesian approach to multidimensional scaling. The package consists of implementations of the methods of Oh and Raftery (2001) <doi:10.1198/016214501753208690>.

License GPL (>= 2)

Depends R (>= 3.5.0)

Imports Rcpp (>= 1.0.7), progress, ggplot2, shinythemes, shiny, gridExtra, rgl, ggpubr

LinkingTo Rcpp, RcppArmadillo

Encoding UTF-8

RoxygenNote 7.1.2

R topics documented:

`bayMDSApp` *Shiny App for exploring the results of* `bmds` *function*

Description

Call Shiny to show the results of Bayesian analysis of multidimensional scaling in a web-based application.

Usage

```
bayMDSApp(out)
```

Arguments

out	an object of class bmds, the output of the bmds function

Value

open Shiny app

Examples

```
data(cityDIST)
out <- bmds(cityDIST, min_p=1, max_p=6 )
if(interactive()){bayMDSApp(out)}
```

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bmds *run bmdsMCMC for various number of dimensions*

Description

Provide object configuration and estimates of parameters, for number of dimensions from min_p to max_p

Usage

```
bmds(DIST,min_p=1, max_p=6,nwarm = 1000,niter = 5000,...)
```

Arguments

DIST	symmetric data matrix of dissimilarity measures for pairs of objects
min_p	minimum number of dimensions for object configuration (default=1)
max_p	maximum number of dimensions for object configuration (default=6)
nwarm	number of iterations for burn-in period in MCMC (default=1000)
niter	number of MCMC iterations after burn-in period (default=5000)
...	arguments to be passed to methods.

Details

Model

The basic model for Bayesian multidimensional scaling given in Oh and Raftery (2001) is as follows. Given the number of dimensions p, we assume that an observed dissimilarity measure follows a truncated multivariate normal distribution with mean equal to Euclidean distance, i.e.,

$d_{ij} \sim N(\delta_{ij}, \sigma^2) I(d_{ij} > 0)$, independently for $i \neq j, i, j = 1, \cdots, n$,

where

- n is the number of objects, i.e, numner of rows in DIST

- d_{ij} is an observed dissimilarity measure between objects i and j
- δ_{ij} is the distance between objects i and j in a p-dimensional Euclidean space, i.e., $\delta_{ij} = \sqrt{\sum_{k=1}^{p}(x_{ik} - x_{jk})^2}$
- $x_i = (x_{i1}, ..., x_{ip})$ denotes the values of the attributes possessed by object i, i.e., the coordinates of object i in a p-dimensional Euclidean space.

Priors

- Prior distribution of x_i is given as a multivariate normal distribution with mean 0 and a diagonal covariance matrix Λ, i.e., $x_i \sim N(0, \Lambda)$, independently for $i = 1, \cdots, n$. Note that the zero mean and diagonal covariance matrix is assumed because Euclidean distance is invariant under translation and rotation of $X = \{x_i\}$.
- Prior distribution of the error variance σ^2 is given as $\sigma^2 \sim IG(a, b)$, the inverse Gamma distribution with mode $b/(a + 1)$.
- Hyperpriors for the elements of $\Lambda = diag(\lambda_1, ..., \lambda_p)$ are given as $\lambda_j \sim IG(\alpha, \beta_j)$, independently for $j = 1, \cdots, p$.
- We assume prior independence among X, Λ, σ^2.

Measure of fit

A measure of fit, called STRESS, is defined as

$$STRESS = \sqrt{\frac{\sum_{i>j}(d_{ij} - \hat{\delta}_{ij})^2}{\sum_{i>j} d_{ij}^2}},$$

where $\hat{\delta}_{ij}$ is the Euclidean distance between objects i and j, computed from the estimated object configuration. Note that the squared $STRESS$ is proportional to the sum of squared residuals, $SSR = \sum_{i>j}(d_{ij} - \hat{\delta}_{ij})^2$.

Value

in `bmds` object

n number of objects, i.e., number of rows in DIST

min_p minimum number of dimensions

max_p maximum number of dimensions

niter number of MCMC iterations

nwarm number of burn-in in MCMC

***** the following lists contains objects from `bmdsMCMC` for number of dimensions from min_p to max_p

x_bmds a list of object configurations

minSSR.L a list of minimum sum of squares of residuals between the observed dissimilarities and the estimated Euclidean distances between pairs of objects

minSSR_id.L a list of the indecies of the iteration corresponding to minimum SSR

stress.L a list of STRESS values

e_sigma.L a list of posterior mean of σ^2

var_sigma.L a list of posterior variance of σ^2

SSR.L a list of posterior samples of SSR

lam.L a list of posterior samples of elements of Λ

sigma.L a list of posterior samples of σ^2, the error variance

del.L a list of posterior samples of δs,Euclidean distances between pairs of objects)

cmds.L a list of object configuration from the classical multidimensional scaling of Togerson(1952)

BMDSp a list of outputs from bmdsMCMC founction for each number of dimensions

References

Oh, M-S., Raftery A.E. (2001). Bayesian Multidimensional Scaling and Choice of Dimension, Journal of the American Statistical Association, 96, 1031-1044.

Torgerson, W.S. (1952). Multidimensional Scaling: I. Theory and Methods, Psychometrika, 17, 401-419.

Examples

```
data(cityDIST)
out <- bmds(cityDIST)
```

`bmdsMCMC` *MCMC for Bayesian multidimensional scaling*

Description

run MCMC algorithm given in Oh and Raftery (2001) and return posterior samples of parameters as well as object configuration and other parameter estimates, for a given number of dimensions p

Usage

```
bmdsMCMC(DIST,p,nwarm = 1000,niter = 5000)
```

Arguments

`DIST`	symmetric matrix of dissimilarity measures between objects
`p`	number of dimensions of object configuration
`nwarm`	number of iterations for burn-in period in MCMC (default=1000)
`niter`	number of MCMC iterations after burn-in period (default=5000)

Value

A list of MCMC results

x_bmds n by p matrix of object configuration that minimizes the sum of squares of residuals(SSR), where n is the number of objects, i.e., n=nrow(DIST)

cmds n by p matrix of object configuration from the classical multidimensional scaling of Togerson(1952)

minSSR minimum of sum of squares of residuals between the observed dissimilarities and the estimated Euclidean distances for pairs of objects

minSSR_id index of the iteration corresponding to minimum SSR

stress STRESS computed from minSSR

e_sigma posterior mean of σ^2

var_sigma posterior variance of σ^2

SSR.L niter dimensional vector of posterior samples of SSR

lam.L niter by p matrix of posterior samples of elements of Λ

sigma.L niter dimensional vector of posterior samples of σ^2

del.L niter by $n(n-1)/2$ matrix of posterior samples of δ, p-dimensional Euclidean distances between pairs of objects

References

Oh, M-S., Raftery A.E. (2001). Bayesian Multidimensional Scaling and Choice of Dimension, Journal of the American Statistical Association, 96, 1031-1044.

Examples

```
data(cityDIST)
result=bmdsMCMC(cityDIST,p=3,nwarm=500,niter=3000)
```

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checkDIST *check the dissimilarity matrix*

Description

check the type of dissimilarity matrix and convert it to a symmetric full matrix for the input of `bmdsMCMC` and `bmds` function

Usage

```
checkDIST(dist, ...)
```

Arguments

`dist`	dissimilarity measures for pairs of objects
`...`	arguments to be passed to methods

Value

a full matrix of dissimilarity measures

Examples

```
x <- matrix(rnorm(100), nrow = 5)
dist(x)
checkDIST(dist(x))
```

cityDIST *Airline distances between cities*

Description

Airline distances between 30 principal cities of the world. Cities are located on the surface of the earth, a three-dimensional sphere, and airplanes travel on the surface of the earth.

References

Hartigan, J.A. (1975), Clustering Algorithms, Wiley, New York.

Examples

```
data(cityDIST)
```

distRcpp *calculate Euclidean distances*

Description

calculate Euclidean distances between rows of matrix X

Usage

```
distRcpp(X)
```

Arguments

X	data matrix

Value

distance matrix

Examples

```
x <- matrix(rnorm(100), nrow = 5)
distRcpp(x)
```

MDSIC *compute and plot MDSIC*

Description

compute and plot MDSIC, a Bayesian selection criterion, given in Oh and Raftery (2001) based on the output of the function bmds

Usage

```
MDSIC(x, plot = TRUE, ...)
```

Arguments

x	an object of class bmds, the output of the function bmds
plot	TRUE/FALSE, if TRUE plot the number of dimensions versus MDSIC (default=TRUE)
...	arguments to be passed to methods

Details

Notes To compute MDSIC, output of the function bmds for min_p=1 is needed for sequential calculation of MDSIC.

Value

a list of MDSIC results

mdsic MDSIC, for p =1,..,max_p

llike log likelihood term in MDSIC, for p=1,...,max_p

penalty penalty term in MDSIC, for p=1,...,max_p

References

Oh, M-S., Raftery A.E. (2001). Bayesian Multidimensional Scaling and Choice of Dimension, Journal of the American Statistical Association, 96, 1031-1044.

Examples

```
data(cityDIST)
out <- bmds(cityDIST, min_p=1, max_p=5 )
MDSIC(out)
```

plotDelDist *plot Delta vs DIST*

Description

plot Delta (estimated Euclidean distance from bmds) vs DIST (observed dissimilarity measure) for pairs of objects

Usage

```
plotDelDist(out)
```

Arguments

out	the output of the function bmdsMCMC

Value

plot of delta vs. dist

Examples

```
data(cityDIST)
result <- bmdsMCMC(cityDIST,p=3,nwarm=500,niter=3000)
plotDelDist(result)
```

plotObj *plot object configuration*

Description

plot object configuration in a Euclidean space of two selected dimensions

Usage

```
plotObj(out, ...)
```

Arguments

out	the output of the function bmdsMCMC
...	arguments to be passed to methods

Value

plot of object configuration

Examples

```
data(cityDIST)
result <- bmdsMCMC(cityDIST,p=3,nwarm=500,niter=3000)
plotObj(result)
```

`plotTrace` *trace plots of MCMC samples*

Description

plot trace plots of MCMC samples of parameters for visual inspection of MCMC convergence

Usage

```
plotTrace(out, para = c("del"), linecolor = "blue", ...)
```

Arguments

`out`	the output of the function `bmdsMCMC`
`para`	names of the parameters for trace plots. It should be any subvector of c("del","sigma", "lambda") (default=c("del"))
`linecolor`	line color. The default color is blue.
`...`	arguments to be passed to methods

Details

Notes

- If "del" is in para, trace plots of the Euclidean distances from 4 randomly selected pairs will be given
- If "lambda" is in para, trace plots of the first four elements of Lambda, the diagonal prior variance of objects, will be given
- If "sigma" is in para, trace plot and ACF(Auto Correlation Function) plot of sigma, the error-variance will be given

Value

trace plots of delta, sigma and lambda

Examples

```
data(cityDIST)
result <- bmdsMCMC(cityDIST,p=3,nwarm=500,niter=3000)
plotTrace(result,para=c("del","sigma", "lambda"))
```

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