

Package: BoltzMM (via r-universe)

September 5, 2024

Type Package

Title Boltzmann Machines with MM Algorithms

Version 0.1.4

Author Andrew Thomas Jones, Hien Duy Nguyen, and Jessica Juanita Bagnall

Maintainer Andrew Thomas Jones <andrewthomasjones@gmail.com>

Description Provides probability computation, data generation, and model estimation for fully-visible Boltzmann machines. It follows the methods described in Nguyen and Wood (2016a) <doi:10.1162/NECO_a_00813> and Nguyen and Wood (2016b) <doi:10.1109/TNNLS.2015.2425898>.

License GPL-3

Encoding UTF-8

LazyData true

LinkingTo Rcpp, RcppArmadillo, BH

Imports Rcpp

Depends R (>= 2.10)

RoxygenNote 7.1.1

Suggests testthat, knitr, rmarkdown, bnstruct

Repository https://andrewthomasjones.r-universe.dev

RemoteUrl https://github.com/andrewthomasjones/boltzmm

RemoteRef HEAD

RemoteSha 0d07f07286e83d945ddba85560c2ad58e9cfc7ee

Contents

allpfvbm	2
BoltzMM	3
fitfvbm	3
fvbmcov	4

fvbmHess	6
fvbmpartiald	7
fvbmstderr	8
fvbmtests	9
log_pl_calc	10
marginpfvbm	10
pfvbm	11
rfvbm	12
senate	13

Index	14
--------------	-----------

allpfvbm	<i>Probability mass function of a fully-visible Boltzmann machine evaluated for all possible vectors.</i>
----------	---

Description

Compute the probability of all 2^n strings of $n > 1$ binary spin variables (i.e. each element is -1 or 1) arising from a fully-visible Boltzmann machine with some specified bias vector and interaction matrix.

Usage

```
allpfvbm(bvec, Mmat)
```

Arguments

bvec	Vector of length n containing real valued bias parameters.
Mmat	Symmetric n by n matrix, with zeros along the diagonal, containing the interaction parameters.

Value

A vector of the probabilities of all 2^n binary spin vectors under a fully-visible Boltzmann machine with bias vector `bvec` and interaction matrix `Mmat`. Probabilities are reported in ascending order of the binary strings; i.e for $n=2$ the reporting order is (-1,1), (-1,-1), (1,-1), and (1,1).

Author(s)

Andrew T. Jones and Hien D. Nguyen

References

H.D. Nguyen and I.A. Wood (2016), Asymptotic normality of the maximum pseudolikelihood estimator for fully-visible Boltzmann machines, IEEE Transactions on Neural Networks and Learning Systems, vol. 27, pp. 897-902.

Examples

```
# Compute the probability of every length n=3 binary spin vector under bvec and Mmat.
bvec <- c(0,0.5,0.25)
Mmat <- matrix(0.1,3,3) - diag(0.1,3,3)
allpfvbm(bvec,Mmat)
```

BoltzMM

BoltzMM: A package for probability computation, data generation, and model estimation of fully-visible Boltzmann machines.

Description

The BoltzMM package allows for computation of probability mass functions of fully-visible Boltzmann machines via `pfvbm` and `allpfvbm`. Random data can be generated using `rfvbm`. Maximum pseudolikelihood estimation of parameters via the MM algorithm can be conducted using `fitfvbm`. Computation of partial derivatives and Hessians can be performed via `fvbmpartiald` and `fvbmHessian`. Covariance estimation and normal standard errors can be computed using `fvbmcov` and `fvbmstderr`.

Author(s)

Andrew T. Jones and Hien D. Nguyen

References

H.D. Nguyen and I.A. Wood (2016), Asymptotic normality of the maximum pseudolikelihood estimator for fully-visible Boltzmann machines, *IEEE Transactions on Neural Networks and Learning Systems*, vol. 27, pp. 897-902.

H.D. Nguyen and I.A. Wood (2016), A block successive lower-bound maximization algorithm for the maximum pseudolikelihood estimation of fully visible Boltzmann machines, *Neural Computation*, vol 28, pp. 485-492.

fitfvbm

Maximum pseudolikelihood estimation of a fully-visible Boltzmann machine.

Description

Estimates the bias vector and interaction matrix of a fully-visible Boltzmann machine via maximum pseudolikelihood estimation using an MM algorithm.

Usage

```
fitfvbm(data, bvec, Mmat, delta_crit = 0.001, max_it = 1000L)
```

Arguments

<code>data</code>	An N by n matrix, where each of the N rows contains a length n string of spin variables (i.e. each element is -1 or 1).
<code>bvec</code>	Initial estimate for a vector of length n containing real valued bias parameters.
<code>Mmat</code>	Initial estimate for a symmetric n by n matrix, with zeros along the diagonal, containing the interaction parameters.
<code>delta_crit</code>	Real threshold value for the convergence criterion, based on the relative change in the Euclidean distance of parameter estimates from consecutive iterations.
<code>max_it</code>	Integer value indicating the maximum number of iterations that the algorithm is to run for.

Value

A list containing 4 objects: the final log-pseudolikelihood value `pll`, a vector containing the estimate of the bias parameters `bvec`, a matrix containing the estimate of the interaction parameters `Mmat`, and the number of algorithm iterations `itt`.

Author(s)

Andrew T. Jones and Hien D. Nguyen

References

H.D. Nguyen and I.A. Wood (2016), A block successive lower-bound maximization algorithm for the maximum pseudolikelihood estimation of fully visible Boltzmann machines, *Neural Computation*, vol 28, pp. 485-492

Examples

```
# Generate num=1000 random strings of n=3 binary spin variables under bvec and Mmat.
num <- 1000
bvec <- c(0,0.5,0.25)
Mmat <- matrix(0.1,3,3) - diag(0.1,3,3)
data <- rfvbm(num,bvec,Mmat)
# Fit a fully visible Boltzmann machine to data, starting from parameters bvec and Mmat.
fitfvbm(data,bvec,Mmat)
```

fvbmcov

Sandwich estimator of the covariance matrix for a fitted fully-visible Boltzmann machine.

Description

Computes the sandwich estimator of the covariance matrix for a maximum pseudolikelihood estimated fully-visible Boltzmann machine.

Usage

```
fvbmcov(data, model, fvbmHess)
```

Arguments

<code>data</code>	An N by n matrix, where each of the N rows contains a length n string of spin variables (i.e. each element is -1 or 1).
<code>model</code>	List generated from <code>fitfvbm</code> .
<code>fvbmHess</code>	A function that computes the Hessian of the parameter elements. Currently, the only implemented method is the default <code>fvbmHess</code> function.

Value

The $n + \text{choose}(n, 2)$ by $n + \text{choose}(n, 2)$ sandwich covariance matrix, estimated using `data` and evaluated at the fitted parameter values provided in `model`. Each row (column) is a unique element of the bias vector and interaction matrix. The rows are arranged in lexicographical order with the bias elements first, followed by the interaction elements. For example, if $n=3$, the order would be `bias[1]`, `bias[2]`, `bias[3]`, `interaction[1,2]`, `interaction[1,3]`, and `interaction[2,3]`.

Author(s)

Andrew T. Jones and Hien D. Nguyen

References

H.D. Nguyen and I.A. Wood (2016), Asymptotic normality of the maximum pseudolikelihood estimator for fully-visible Boltzmann machines, *IEEE Transactions on Neural Networks and Learning Systems*, vol. 27, pp. 897-902.

Examples

```
# Generate num=1000 random strings of n=3 binary spin variables under bvec and Mmat.
num <- 1000
bvec <- c(0, 0.5, 0.25)
Mmat <- matrix(0.1, 3, 3) - diag(0.1, 3, 3)
data <- rfvbm(num, bvec, Mmat)
# Fit a fully visible Boltzmann machine to data, starting from parameters bvec and Mmat.
model <- fitfvbm(data, bvec, Mmat)
# Compute the sandwich covariance matrix using the data and the model.
fvbmcov(data, model, fvbmHess)
```

fvbmHess	<i>Hessian of the log-pseudolikelihood function for a fitted fully-visible Boltzmann machine.</i>
----------	---

Description

Computes the Hessian with respect to all unique parameter elements of the bias vector and interaction matrix of a fully-visible Boltzmann machine, for some random length n string of spin variables (i.e. each element is -1 or 1) and some fitted parameter values.

Usage

```
fvbmHess(data, model)
```

Arguments

data	An N by n matrix, where each of the N rows contains a length n string of spin variables (i.e. each element is -1 or 1).
model	List generated from <code>fitfvbm</code> .

Value

The $n + \text{choose}(n,2)$ by $n + \text{choose}(n,2)$ Hessian matrix, summed over the N rows of `data` and evaluated at the fitted parameter values provided in `model`. Each row (column) is a unique element of the bias vector and interaction matrix. The rows are arranged in lexicographical order with the bias elements first, followed by the interaction elements. For example, if $n=3$, the order would be `bias[1]`, `bias[2]`, `bias[3]`, `interaction[1,2]`, `interaction[1,3]`, and `interaction[2,3]`.

Author(s)

Andrew T. Jones and Hien D. Nguyen

References

H.D. Nguyen and I.A. Wood (2016), Asymptotic normality of the maximum pseudolikelihood estimator for fully-visible Boltzmann machines, *IEEE Transactions on Neural Networks and Learning Systems*, vol. 27, pp. 897-902.

Examples

```
# Generate num=1000 random strings of n=3 binary spin variables under bvec and Mmat.
num <- 1000
bvec <- c(0,0.5,0.25)
Mmat <- matrix(0.1,3,3) - diag(0.1,3,3)
data <- rfvbm(num,bvec,Mmat)
# Fit a fully visible Boltzmann machine to data, starting from parameters bvec and Mmat.
model <- fitfvbm(data,bvec,Mmat)
# Compute the Hessian matrix summed over all num rows of data.
fvbmHess(data,model)
```

fvbpartiald	<i>Partial derivatives of the log-pseudolikelihood function for a fitted fully-visible Boltzmann machine.</i>
-------------	---

Description

Computes the partial derivatives for all unique parameter elements of the bias vector and interaction matrix of a fully-visible Boltzmann machine, for some random length n string of spin variables (i.e. each element is -1 or 1) and some fitted parameter values.

Usage

```
fvbpartiald(data, model)
```

Arguments

data	Vector of length n containing binary spin variables.
model	List generated from <code>fitfvbm</code> .

Value

A list containing 2 objects: a vector containing the partial derivatives corresponding to the bias parameters `bvec`, and a matrix containing the partial derivatives corresponding to the interaction parameters `Mmat`.

Author(s)

Andrew T. Jones and Hien D. Nguyen

References

H.D. Nguyen and I.A. Wood (2016), Asymptotic normality of the maximum pseudolikelihood estimator for fully-visible Boltzmann machines, IEEE Transactions on Neural Networks and Learning Systems, vol. 27, pp. 897-902.

Examples

```
# Generate num=1000 random strings of n=3 binary spin variables under bvec and Mmat.
num <- 1000
bvec <- c(0,0.5,0.25)
Mmat <- matrix(0.1,3,3) - diag(0.1,3,3)
data <- rfvbm(num,bvec,Mmat)
# Fit a fully visible Boltzmann machine to data, starting from parameters bvec and Mmat.
model <- fitfvbm(data,bvec,Mmat)
# Compute the partial derivatives evaluated at the first observation of data.
fvbpartiald(data,model)
```

fvbmstderr	<i>Standard errors for the parameter elements of a fitted fully-visible Boltzmann machine.</i>
------------	--

Description

Computes the normal approximation standard errors from the sandwich estimator of the covariance matrix for a maximum pseudolikelihood estimated fully-visible Boltzmann machine.

Usage

```
fvbmstderr(data, covarmat)
```

Arguments

data	An N by n matrix, where each of the N rows contains a length n string of spin variables (i.e. each element is -1 or 1).
covarmat	A covariance matrix generated from fvbmcov.

Value

A list containing 2 objects: a vector containing the standard errors corresponding to the bias parameters `bvec_se`, and a matrix containing the standard errors corresponding to the interaction parameters `Mmat_se`.

Author(s)

Andrew T. Jones and Hien D. Nguyen

References

H.D. Nguyen and I.A. Wood (2016), Asymptotic normality of the maximum pseudolikelihood estimator for fully-visible Boltzmann machines, *IEEE Transactions on Neural Networks and Learning Systems*, vol. 27, pp. 897-902.

Examples

```
# Generate num=1000 random strings of n=3 binary spin variables under bvec and Mmat.
num <- 1000
bvec <- c(0,0.5,0.25)
Mmat <- matrix(0.1,3,3) - diag(0.1,3,3)
data <- rfvbm(num,bvec,Mmat)
# Fit a fully visible Boltzmann machine to data, starting from parameters bvec and Mmat.
model <- fitfvbm(data,bvec,Mmat)
# Compute the sandwich covariance matrix using the data and the model.
covarmat <- fvbmcov(data,model,fvbmHess)
# Compute the standard errors of the parameter elements according to a normal approximation.
fvbmstderr(data,covarmat)
```


fvbmtests

*Hypothesis testing for a fully-visible Boltzmann machine.***Description**

Tests the hypothesis that the true bias and interaction parameter values are those in `nullmodel`, given data and `model`.

Usage

```
fvbmtests(data, model, nullmodel)
```

Arguments

<code>data</code>	An N by n matrix, where each of the N rows contains a length n string of spin variables (i.e. each element is -1 or 1).
<code>model</code>	List generated from <code>fitfvbm</code> .
<code>nullmodel</code>	A list containing two elements: a vector of length n <code>bvec</code> , and an n by n matrix <code>Mmat</code> . A list generated by <code>fitfvbm</code> is also sufficient.

Value

A list containing 4 objects: a vector containing the z-scores corresponding to the bias parameters `bvec_z`, a vector containing the p-values corresponding to the bias parameters `bvec_p`, a matrix containing the z-scores corresponding to the interaction parameters `Mmat_z`, and a matrix containing the standard errors corresponding to the interaction parameters `Mmat_p`.

Author(s)

Andrew T. Jones and Hien D. Nguyen

References

H.D. Nguyen and I.A. Wood (2016), Asymptotic normality of the maximum pseudolikelihood estimator for fully-visible Boltzmann machines, *IEEE Transactions on Neural Networks and Learning Systems*, vol. 27, pp. 897-902.

Examples

```
# Generate num=1000 random strings of n=3 binary spin variables under bvec and Mmat.
num <- 1000; bvec <- c(0,0.5,0.25); Mmat <- matrix(0.1,3,3) - diag(0.1,3,3);
data <- rfvbm(num,bvec,Mmat)
# Fit a fully visible Boltzmann machine to data, starting from parameters bvec and Mmat.
model <- fitfvbm(data,bvec,Mmat)

#Propose a null hypothesis model
nullmodel <- list(bvec = c(0,0,0), Mmat = matrix(0,3,3))
```

```
# Compute z-scores
fvbmtests(data,model,nullmodel)
```

log_pl_calc	<i>Compute the log pseudolikelihood</i>
-------------	---

Description

Compute the log pseudolikelihood

Usage

```
log_pl_calc(data, L)
```

Arguments

data	An N by n matrix, where each of the N rows contains a length n string of spin variables (i.e. each element is -1 or 1).
List	A list where

Value

The the log pseudolikelihood of [].

Author(s)

Andrew T. Jones and Hien D. Nguyen

marginpfvbm	<i>Marginal probability function for a fully-visible Boltzmann machine.</i>
-------------	---

Description

Computes the marginal probabilities (for values = +1 in each coordinate) under under some specified bias vector and interaction matrix, specified by bvec and Mmat, respectively.

Usage

```
marginpfvbm(bvec, Mmat)
```

Arguments

bvec	Vector of length n containing real valued bias parameters.
Mmat	Symmetric n by n matrix, with zeros along the diagonal, containing the interaction parameters.

Value

Vector of length n containing the marginal probabilities of +1 in each coordinate.

Author(s)

Andrew T. Jones and Hien D. Nguyen

References

H.D. Nguyen and I.A. Wood (2016), Asymptotic normality of the maximum pseudolikelihood estimator for fully-visible Boltzmann machines, *IEEE Transactions on Neural Networks and Learning Systems*, vol. 27, pp. 897-902.

Examples

```
#Compute the marginal probabilities under bvec and Mmat.
# Set the parameter values
bvec <- c(0,0.5,0.25)
Mmat <- matrix(0.1,3,3) - diag(0.1,3,3)
marginpfvbm(bvec,Mmat)
```

pfvbm

Probability mass function of a fully-visible Boltzmann machine evaluated for an individual vector.

Description

Compute the probability of a string of $n > 1$ binary spin variables (i.e. each element is -1 or 1) arising from a fully-visible Boltzmann machine with some specified bias vector and interaction matrix.

Usage

```
pfvbm(xval, bvec, Mmat)
```

Arguments

xval	Vector of length n containing binary spin variables.
bvec	Vector of length n containing real valued bias parameters.
Mmat	Symmetric n by n matrix, with zeros along the diagonal, containing the interaction parameters.

Value

The probability of the random string `xval` under a fully-visible Boltzmann machine with bias vector `bvec` and interaction matrix `Mmat`.

Author(s)

Andrew T. Jones and Hien D. Nguyen

References

H.D. Nguyen and I.A. Wood (2016), Asymptotic normality of the maximum pseudolikelihood estimator for fully-visible Boltzmann machines, IEEE Transactions on Neural Networks and Learning Systems, vol. 27, pp. 897-902.

Examples

```
# Compute the probability of the vector xval=(-1,1,-1), under bvec and Mmat.
xval <- c(-1,1,-1)
bvec <- c(0,0.5,0.25)
Mmat <- matrix(0.1,3,3) - diag(0.1,3,3)
pfvbm(xval,bvec,Mmat)
```

 rfvbm

Random data generation from a fully-visible Boltzmann machine.

Description

Generate N random strings of n>1 binary spin variables (i.e. each element is -1 or 1) arising from a fully-visible Boltzmann machine with some specified bias vector and interaction matrix.

Usage

```
rfvbm(num, bvec, Mmat)
```

Arguments

num	Number N of random strings to be generated.
bvec	Vector of length n containing real valued bias parameters.
Mmat	Symmetric n by n matrix, with zeros along the diagonal, containing the interaction parameters.

Value

An N by n matrix, where each row contains a random spin variable string from a fully-visible Boltzmann machine with bias vector bvec and interaction matrix Mmat.

Note

The function `allpfvbm` must be called each time this function is run. Thus, it is much more efficient to generate N strings all at once, than to generate strings one at a time.

Author(s)

Andrew T. Jones and Hien D. Nguyen

References

H.D. Nguyen and I.A. Wood (2016), Asymptotic normality of the maximum pseudolikelihood estimator for fully-visible Boltzmann machines, IEEE Transactions on Neural Networks and Learning Systems, vol. 27, pp. 897-902.

Examples

```
# Generate num=10 random strings of n=3 binary spin variables under bvec and Mmat.  
num <- 10  
bvec <- c(0,0.5,0.25)  
Mmat <- matrix(0.1,3,3) - diag(0.1,3,3)  
rfvbm(num,bvec,Mmat)
```

senate

Senate voting data from the 45th Australian Parliament.

Description

A dataset he data from the first sitting of the Senate of the 45th Australian Parliament, until the final sitting of the year 2016. The first division during this period was conducted on the 31st of August 2016, and the last division was performed on the 1st of December 2016. In total, 147 divisions were performed during this period.

Each row represents a division(vote), each column is a party or independent. Data is either "Yes" or "No" depending on the vote. Absences and abstentions are left as NA. See <https://hal.archives-ouvertes.fr/hal-01927188v1> for details of data preparation.

Usage

```
data(senate)
```

Format

A data frame with 147 rows (votes) and 9 variables (parties).

Author(s)

Jessica J. Bagnall

Source

www.aph.gov.au/Parliamentary_Business/Statistics/Senate_StatsNet/General/divisions

Examples

```
dim(senate)
```

Index

- * **datasets**
 - senate, [13](#)
- allpfvbm, [2](#)
- BoltzMM, [3](#)
- fitfvbm, [3](#)
- fvbmcov, [4](#)
- fvbmHess, [6](#)
- fvbmpartiald, [7](#)
- fvbmstderr, [8](#)
- fvbmtests, [9](#)
- log_pl_calc, [10](#)
- marginpfvbm, [10](#)
- pfvbm, [11](#)
- rfvbm, [12](#)
- senate, [13](#)