

# Package ‘bayesMRM’

July 22, 2025

**Type** Package

**Title** Bayesian Multivariate Receptor Modeling

**Version** 2.4.0

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**Description** Bayesian analysis of multivariate receptor modeling. The package consists of implementations of the methods of Park and Oh (2015) <doi:10.1016/j.chemolab.2015.08.021>. The package uses 'JAGS'(Just Another Gibbs Sampler) to generate Markov chain Monte Carlo samples of parameters.

**Date** 2022-12-14

**Depends** R (>= 4.0.0)

**License** GPL (>= 2)

**Encoding** UTF-8

**Imports** rjags,coda,ggplot2,grDevices,graphics,gridExtra,rgl,shiny,shinythemes

**Suggests** stats

**RoxygenNote** 7.2.1

**NeedsCompilation** no

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**Repository** CRAN

**Date/Publication** 2022-12-14 07:30:05 UTC

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bayesMRMApp	<i>Shiny App for exploring the results of Bayesian multivariate receptor modeling</i>
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## Description

Call Shiny to show the results of Bayesian analysis of multivariate receptor modeling in a web-based application. This object contains

- plots of the posterior means and 95% posterior intervals of parameters in an object of class `bmrm`.
- tables of the posterior means of parameters in an object of class `bmrm`.
- tables of the posterior quantiles of parameters in an object of class `bmrm`, for `prob=(0.025, 0.05, 0.25, 0.5, 0.75, 0.95, 0.975)`.
- tables of convergence diagnostics of parameters in an object of class `bmrm`.
- 3-dimensional dynamic principal component plots of data (Y) and source profiles (rows of the estimated source composition matrix P) in an object of class `bmrm`. The plot can be rotated by moving the cursor.
- trace plots and ACF plots of the first 6 elements of a parameter in an object of class `bmrm`.

## Usage

```
bayesMRMApp(x)
```

## Arguments

x                    an object of class `bmrm`, the output of the `bmrm` function

## Value

shiny App

**Description**

Generate posterior samples of the source composition matrix  $P$ , the source contribution matrix  $A$ , and the error variance  $\Sigma$  using 'JAGS', and computes estimates of  $A, P, \Sigma$ .

**Usage**

```
bmrn(Y, q, muP, errdist="norm", df=4,
      varP.free=100, xi=NULL, Omega=NULL,
      a0=0.01, b0=0.01,
      nAdapt=1000, nBurnIn=5000, nIter=5000, nThin=1,
      P.init=NULL, A.init=NULL, Sigma.init=NULL,...)
```

**Arguments**

Y	data matrix
q	number of sources. It must be a positive integer.
muP	(q,ncol(Y))-dimensional prior mean matrix for the source composition matrix $P$ , where $q$ is the number of sources. Zeros need to be assigned to prespecified elements of $\mu P$ to satisfy the identifiability condition C1. For the remaining free elements, any nonnegative numbers (between 0 and 1 preferably) can be assigned. If no or an insufficient number of zeros are preassigned in $\mu P$ , estimation can still be performed but the resulting estimates may be subject to rotational ambiguities. (default=0.5 for nonzero elements).
errdist	error distribution: either "norm" for normal distribution or "t" for t distribution (default="norm")
df	degrees of freedom of a t-distribution when errdist="t" (default=4)
varP.free	scalar value of the prior variance of the free (nonzero) elements of the source composition matrix $P$ (default=100)
xi	prior mean vector of the $q$ -dimensional source contribution vector at time $t$ (default=vector of 1's)
Omega	diagonal matrix of the prior variance of the $q$ -dimensional source contribution vector at time $t$ (default=identity matrix)
a0	shape parameter of the Inverse Gamma prior of the error variance (default=0.01)
b0	scale parameter of the Inverse Gamma prior of the error variance (default=0.01)
nAdapt	number of iterations for adaptation in 'JAGS' (default=1000)
nBurnIn	number of iterations for the burn-in period in MCMC (default=5000)
nIter	number of iterations for monitoring samples from MCMC (default=5000). nIter samples are saved in each chain of MCMC.
nThin	thinning interval for monitoring samples from MCMC (default=1)

P.init	initial value of the source composition matrix P. If omitted, zeros are assigned to the elements corresponding to zero elements in muP and the nonzero elements of P.init will be randomly generated from a uniform distribution.
A.init	initial value of the source contribution matrix A. If omitted, it will be calculated from Y and P.init.
Sigma.init	initial value of the error variance. If omitted, it will be calculated from Y, A.init and P.init.
...	arguments to be passed to methods

## Details

### Model

The basic model for Bayesian multivariate receptor model is as follows:

$$Y_t = A_t P + E_t, t = 1, \dots, T,$$

where

- $Y_t$  is a vector of observations of  $J$  variables at time  $t, t = 1, \dots, T$ .
- $P$  is a  $q \times J$  source composition matrix in which the  $k$ -th row represents the  $k$ -th source composition profiles,  $k = 1, \dots, q, q$  is the number of sources.
- $A_t$  is a  $q$  dimensional source contribution vector at time  $t, t = 1, \dots, T$ .
- $E_t = (E_{t1}, \dots, E_{tJ})$  is an error term for the  $t$ -th observations, following  $E_t \sim N(0, \Sigma)$  or  $E_t \sim t_{df}(0, \Sigma)$ , independently for  $j = 1, \dots, J$ , where  $\Sigma = \text{diag}(\sigma_1^2, \dots, \sigma_J^2)$ .

### Priors

- Prior distribution of  $A_t$  is given as a truncated multivariate normal distribution,
  - $A_t \sim N(\xi, \Omega)I(A_t \geq 0)$ , independently for  $t = 1, \dots, T$ .
- Prior distribution of  $P_{kj}$  (the  $(k, j)$ -th element of the source composition matrix  $P$ ) is given as
  - $P_{kj} \sim N(\text{muP}_{kj}, \text{varP.free})I(P_{kj} \geq 0)$ , for free (nonzero)  $P_{kj}$ ,
  - $P_{kj} \sim N(0, 1e-10)I(P_{kj} \geq 0)$ , for zero  $P_{kj}$ , independently for  $k = 1, \dots, q; j = 1, \dots, J$ .
- Prior distribution of  $\sigma_j^2$  is  $IG(a0, b0)$ , i.e.,
  - $1/\sigma_j^2 \sim \text{Gamma}(a0, b0)$ , having mean  $a0/b0$ , independently for  $j = 1, \dots, J$ .

### Notes

- We use the prior  $P_{kj} \sim N(0, 1e-10)I(P_{kj} \geq 0)$  that is practically equal to the point mass at 0 to simplify the model building in 'JAGS'.
- The MCMC samples of A and P are post-processed (rescaled) before saving so that  $\sum_{j=1}^J P_{kj} = 1$  for each  $k = 1, \dots, q$  (the identifiability condition C3 of Park and Oh (2015)).

**Value**

in bmrn object

**nsource** number of sources

**nobs** number of observations in data Y

**nvar** number of variables in data Y

**Y** observed data matrix

**muP** prior mean of the source composition matrix P

**errdist** error distribution

**df** degrees of freedom when errdist="t"

**A.hat** posterior mean of the source contribution matrix A

**P.hat** posterior mean of the source composition matrix P

**Sigma.hat** posterior mean of the error variance Sigma

**A.sd** posterior standard deviation of the source contribution matrix A

**P.sd** posterior standard deviation of the source composition matrix P

**Sigma.sd** posterior standard deviation of the error variance Sigma

**A.quantiles** posterior quantiles of A for prob=(0.025, 0.05, 0.25, 0.5, 0.75, 0.95, 0.975)

**P.quantiles** posterior quantiles of P for prob=(0.025, 0.05, 0.25, 0.5, 0.75, 0.95, 0.975)

**Sigma.quantiles** posterior quantiles of Sigma for prob=(0.025, 0.05, 0.25, 0.5, 0.75, 0.95, 0.975)

**Y.hat** predicted value of Y computed from A.hat\*P.hat

**residual** Y-Y.hat

**codaSamples** MCMC posterior samples of A, P, and  $\Sigma$  in class "mcmc.list"

**nIter** number of MCMC iterations per chain for monitoring samples from MCMC

**nBurnIn** number of iterations for the burn-in period in MCMC

**nThin** thinning interval for monitoring samples from MCMC

**References**

Park, E.S. and Oh, M-S. (2015), Robust Bayesian Multivariate Receptor Modeling, Chemometrics and intelligent laboratory systems, 149, 215-226.

Plummer, M. 2003. JAGS: A program for analysis of Bayesian graphical models using Gibbs sampling. Proceedings of the 3rd international workshop on distributed statistical computing, pp. 125. Technische Universit at Wien, Wien, Austria.

Plummer, M. 2015. 'JAGS' Version 4.0.0 user manual.

**Examples**

```
data(Elpaso); Y=Elpaso$Y ; muP=Elpaso$muP ; q=nrow(muP)
out.Elpaso <- bmrn(Y,q,muP)
summary(out.Elpaso)
plot(out.Elpaso)
```

convdiag\_bmm

*Convergence Diagnostics on MCMC samples in bmm***Description**

Compute convergence diagnostics of Geweke (1992), Heidelberger and Welch (1983), Raftery and Lewis(1992).

**Usage**

```
convdiag_bmm(x , var="P", convdiag="geweke",print=TRUE,...)
```

**Arguments**

x	an object of class bmm, the output of the bmm function
var	name of a variable to which convergence diagnostics apply. It should be one of "A" (source contribution matrix), "P" (source composition or profile matrix), "Sigma" (error variance).
convdiag	vector of convergence diagnostic methods. It should be any subvector of ("geweke", "heidel", "raftery" ) (default="geweke").
print	TRUE/FALSE, print convergence diagnostics results (default=TRUE)
...	arguments to be passed to methods

**Details**

Geweke's convergence diagnostic for Markov chains is based on a test for equality of the means of the first and last part of a Markov chain (by default the first 10% and the last 50%). If the samples are drawn from the stationary distribution of the chain, the two means should be equal and Geweke's statistic has an asymptotically standard normal distribution. We use the function `geweke.diag` in **cod**a package (with default option) which provides the test statistics (standard Z-scores) and the upper bound of and p-values.

Heidelberger and Welch's convergence diagnostic tests the null hypothesis that the sampled values come from a stationary distribution. The test is successively applied, firstly to the whole chain, then after discarding the first 10%, 20%, ... of the chain until either the null hypothesis is accepted, or 50% of the chain has been discarded. We use the function `heidel.diag` (with default option) which provides the stationary test results and p-values.

Raftery and Lewis's diagnostic estimates the minimum number of iterations, burn-in, thinning interval for zero autocorrelation, satisfying specified conditions regarding quantile  $q$  of parameters of interest. The conditions are specified by a posterior quantile  $q$  of parameters, an acceptable tolerance (accuracy)  $r$  for  $q$ , a probability  $s$  of being within the interval  $q - r, q + r$ . We use the function `raftery.diag` (with default option).

**Value**

A list of convergence diagnostics results

**convdiag** selected convergence diagnostic methods

**geweke** Geweke's z-scores and p-values if convdiag includes "geweke", NULL if convdiag does not include "geweke"

**heidel** Heidelberger and Welch's stationary test results and p-values if convdiag includes "heidel"; NULL if convdiag does not include "heidel"

**raftery** Raftery and Lewis's estimates of burn-in, minimum number of iterations, and thinning if convdiag includes "raftery"; NULL if convdiag does not include "raftery"

**References**

Geweke, J.(1992) Evaluating the accuracy of sampling-based approaches to calculating posterior moments. In Bayesian Statistics 4 (ed JM Bernardo, JO Berger, AP Dawid and AFM Smith). Clarendon Press.

Heidelberger P, and Welch PD. (1981) A spectral method for confidence interval generation and run length control in simulations. Comm. ACM. 24, 233-245.

Heidelberger P. and Welch PD.(1983) Simulation run length control in the presence of an initial transient. Opns Res., 31, 1109-44,Oxford, UK.

Plummer, M., Best, N., Cowles, K. and Vines K. (2006) CODA: Convergence Diagnosis and Output Analysis for MCMC, R News, Vol 6, pp. 7-11.

Raftery, A.E. and Lewis, S.M. (1992). One long run with diagnostics: Implementation strategies for Markov chain Monte Carlo. Statistical Science, 7, 493-497.

Raftery, A.E. and Lewis, S.M. (1995). The number of iterations, convergence diagnostics and generic Metropolis algorithms. In Practical Markov Chain Monte Carlo (W.R. Gilks, D.J. Spiegelhalter and S. Richardson, eds.). London, U.K.: Chapman and Hall.

**Examples**

```
data(Elpaso)
Y=Elpaso$Y ; muP=Elpaso$muP
q=nrow(muP)
out.Elpaso <- bmr(Y,q,muP, nAdapt=1000,nBurnIn=5000,nIter=5000,nThin=1)
conv1<-convdiag_bmr(out.Elpaso,var="P",convdiag="raftery" )
conv2<-convdiag_bmr(out.Elpaso,var="A", convdiag="geweke")
conv3<-convdiag_bmr(out.Elpaso,var="Sigma", convdiag=c("geweke","heidel"))
conv4<-convdiag_bmr(out.Elpaso,var="Sigma", convdiag=c("geweke","heidel", "raftery"))
```

---

Elpaso

*PM2.5 speciation data from El Paso, Texas, USA.*

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## Description

The data frame has the following components:

- $Y$  224 by 15 matrix of 224 observations on 15 PM2.5 species. PM 2.5 was measured every three days during the time period of 1/2/2006 ~ 4/7/2009 from the Chamizal station in the city of El Paso, USA. Out of the 58 original PM 2.5 species, 15 species were selected. After removing any observations with missig values, the final data consists of 224 complete observatins on the following 15 PM2.5 species:

**Al** Aluminum

**Ca** Calcium

**Cl2** Chlorine

**EC** EC CSN

**Fe** Iron

**K\_p** Potassium ion

**Mg** Magnanese

**NV\_NO3** Non-volatile nitrate

**NH4\_p** Ammonium ion

**Na** Sodium

**OC** OC CSN unadjusted

**SO4** Sulfate

**Si** Silicon

**Ti** Titanium

**Zn** Zinc

- $\mu P$  4 by 15 matrix of the prior mean of the source composition matrix  $P$  for data. Zero values are assigned for some elements of  $\mu P$  to satisfy the identifiability conditions C1-C2 in Park and Oh (2015). The remaining nonzero elements of  $\mu P$  have value 0.5. Note that the number of sources (the number of rows in  $\mu P$ ) is presumed to be 4 here.

## References

Park, E.S. and Oh, M-S. (2016), Bayesian Quantile Multivariate Receptor Modeling, Chemometrics and intelligent laboratory systems, 159, 174-180.

## Examples

```
data(Elpaso)
Y=Elpaso$Y
muP=Elpaso$muP
```



---

idcond_check	<i>Check the identifiability conditions</i>
--------------	---

---

**Description**

Check the identifiability conditions C1-C2 of Park and Oh (2015).

**Usage**

```
idCond_check(P)
```

**Arguments**

P source composition matrix in multivariate receptor model

**Value**

idCond TRUE if all the conditions are satisfied, FALSE otherwise

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pcplot	<i>Principal component plot</i>
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---

**Description**

Draw principal component plots of data (Y) and source profiles (rows) of the estimated source composition matrix  $\hat{P}$  (and  $P_0$  if there is another source composition matrix  $P_0$  to compare, e.g.,  $P_0$  could be the true P in simulation or  $P_0$  could be another estimate of P)

**Usage**

```
pcplot(x, P0, G3D=FALSE, ...)
```

**Arguments**

x an object of class bmm, the output from the function bmm  
P0 estimated value of P (in simulation it can be the true value of P)  
G3D TRUE/FALSE, dynamic 3D plot (default=FALSE)  
... arguments to be passed to methods

**Value**

plot

**Examples**

```

data(Elpaso)
Y=Elpaso$Y ; muP=Elpaso$muP
q=nrow(muP)
out.Elpaso <- bmrm(Y,q,muP, nAdapt=1000,nBurnIn=5000,nIter=5000,nThin=1)
pcplot(out.Elpaso)
pcplot(out.Elpaso,G3D=TRUE)

```

---

plot.bmrm

---

*Produce plots of the parameter estimates*


---

**Description**

Produce plots of the estimated posterior mean and 95% posterior intervals of A,P, Sigma based on the MCMC samples in bmrm.

**Usage**

```

## S3 method for class 'bmrm'
plot(x, type = "both", ...)

```

**Arguments**

x	an object of class bmrm, the output of the function bmrm
type	name of a variable (default="P"). It should be one of "P"(source composition or profile matrix P), "A"(source contribution matrix A), "both" (both P and A), "Sigma" (error variance).
...	arguments to be passed to methods

**Details**

The following types of plots are drawn depending on the selected parameters:

- P: bar plots of the posterior means with 95% posterior intervals of elements for each row of P
- A: time series plots of posterior means with 95% posterior intervals elements for each column of A
- Sigma: posterior means with error bars for 95% posterior intervals of elements of Sigma

**Value**

plot

---

summary.bmrn	<i>Summarize the output of the bmrn function</i>
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---

**Description**

An S3 method that summarizes the output of the bmrn function in an object of class bmrn. This object contains the posterior mean, the posterior standard deviation, and (0.025, 0.05, 0.25, 0.5, 0.75, 0.95, 0.975) posterior quantiles of A, P,  $\Sigma$ . It also contains other relevant information about the MCMC procedure such as the burn-in iterations, the number of MCMC chains, etc.

**Usage**

```
## S3 method for class 'bmrn'
summary(object, digits = 3, ...)
```

**Arguments**

object	an object of class bmrn, the output of the bmrn function
digits	integer indicating the number of significant digits
...	arguments to be passed to methods

**Value**

summary of bmrn class (output of bmrn function)

---

trace_ACF_plot	<i>Trace and/or ACF plots of elements of a variable in bmrn object</i>
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---

**Description**

Produce trace and Auto-Correlation Function plots (along with Effective sample size) of MCMC samples of elements of A, nonzero elements of P, elements of Sigma.

**Usage**

```
trace_ACF_plot(x, var="P", ACF=FALSE, nplot=0, irow=1, icol=1, saveFile=FALSE, ...)
```

**Arguments**

x	an object of class bmrn, the output of the bmrn function
var	name of a variable to which the plots apply. It should be one of "A" (source contribution matrix), "P" (source composition matrix), "Sigma" (error variance).
ACF	TRUE/FALSE if TRUE ACF plots will be provided along with effective sample sizes (default: FALSE)

nplot	number of elements of 'var' for trace and/or ACF plots. If 'nplot' is smaller than the total number of elements of 'var' then plots of 'nplot' selected elements will be drawn. Otherwise, trace and/or ACF plots of all elements will be drawn. (default=0 implies that all elements will be selected if var="P" or "Sigma", and the first 12 elements will be selected if var="A")
irow	row index of A/P matrix or index of element of Sigma vector. Plots of 'nplot' elements starting from (irow, icol) element of A/P or elements starting from irow element of Sigma will be drawn (default=1).
icol	column number of A/P matrix. Plots of 'nplot' elements starting from (irow, icol) element of A/P will be drawn (default=1).
saveFile	TRUE/FALSE, save the plots in file ' <i>var</i> '-trace.pdf (default=FALSE)
...	arguments to be passed to methods

**Value**

plot

**Examples**

```
data(Elpaso); Y=Elpaso$Y ; muP=Elpaso$muP ; q=nrow(muP)
out.Elpaso <- bmm(Y,q,muP, nAdapt=1000,nBurnIn=5000,nIter=5000,nThin=1)
trace_ACF_plot(out.Elpaso,"Sigma", ACF=TRUE)
trace_ACF_plot(out.Elpaso,"P", ACF=TRUE)
trace_ACF_plot(out.Elpaso,"A",ACF=TRUE, nplot=12, irow=2, icol=3)
```

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