

# Package ‘BCE’

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**Title** Bayesian composition estimator: estimating sample (taxonomic) composition from biomarker data

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**Depends** R (>= 2.0.1), limSolve

**Description** Function to estimates taxonomic compositions from biomarker data, using a Bayesian approach.

**License** GPL

**LazyData** yes

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**Description**

estimates probability distributions of a sample composition based on an **input ratio matrix**, `Rat`, containing biomarker ratios in (field) samples, and an **input data matrix**, `Dat`, containing the biomarker ratios for several taxonomic groups

**Usage**

```
BCE(Rat, Dat, relsdRat = 0, abssdRat = 0, minRat = 0,
    maxRat = +Inf, relsdDat = 0, abssdDat = 0, tol = 1e-4, tolX = 1e-4,
    positive = 1:ncol(Rat), iter = 100, outputlength = 1000,
    burninlength = 0, jmpRat = 0.01, jmpX = 0.01, unif = FALSE,
    verbose = TRUE, initRat = Rat, initX = NULL, userProb = NULL,
    confInt = 2/3, export = FALSE, file = "BCE")
```

**Arguments**

<code>Rat</code>	initial ratio matrix. Each row of <code>Rat</code> contains the biomarker composition of one taxon. As a result of the Bayesian procedure, this initial ratio matrix will be altered.
<code>Dat</code>	initial data matrix. Each row of <code>Dat</code> contains the biomarker composition of one (field) sample.
<code>relsdRat</code>	relative standard deviation on ratio matrix. Either one number or a matrix with the same dimensions as <code>Rat</code> .
<code>abssdRat</code>	absolute standard deviation on ratio matrix. Either one number or a matrix with the same dimensions as <code>Rat</code> .
<code>minRat</code>	minimum values of ratio matrix. Either one number or a matrix with the same dimensions as <code>Rat</code> .
<code>maxRat</code>	maximum values of ratio matrix. Either one number or a matrix with the same dimensions as <code>Rat</code> .
<code>relsdDat</code>	relative standard deviation on data matrix. Either one number or a matrix with the same dimensions as <code>Dat</code> .
<code>abssdDat</code>	absolute standard deviation on data matrix. Either one number or a matrix with the same dimensions as <code>Dat</code> .
<code>tol</code>	minimum standard deviation for data matrix <code>Dat</code> . One value.
<code>tolX</code>	minimum x values. Used for MCMC initiation. One value.
<code>positive</code>	A vector containing numbers of columns that should contain strictly positive data. Only these columns are rescaled. The other columns (not in <code>positive</code> ) are not rescaled, and can become negative.
<code>iter</code>	number of iterations for MCMC.

<code>outputlength</code>	number of iterations kept in the output.
<code>burninlength</code>	number of initial iterations to be removed from output.
<code>jmpRat</code>	jump length of the ratio matrix <code>Rat</code> (in normal space). Either a number, a vector with length equal to the number of biomarkers (number of columns in <code>Rat</code> ), or a or matrix with the same dimensions as the ratio matrix <code>rat</code> .
<code>jmpX</code>	jump length of the composition matrix (in a simplex). Either one number, a vector of length equal to the number of taxa (number of rows in <code>Rat</code> ) or a matrix with the same dimensions = c(number of taxa, number of field samples).
<code>unif</code>	logical; if TRUE a uniform distribution for ratio matrix is used. This is similar as in <code>chemtax</code> .
<code>verbose</code>	logical; if TRUE, extra information is provided during the run of the function, such as extra warnings, elapsed time and expected time until the end of the MCMC.
<code>initRat</code>	ratio matrix used to start the markov chain: defaults to the initial ratio matrix.
<code>initX</code>	composition matrix used to start the markov chain: default the LSEI solution of $Ax=B$ .
<code>userProb</code>	function taking two arguments: ratio matrix <code>RAT</code> and composition matrix <code>X</code> , and returning the posterior probability. Dependence of the probability on the data should be incorporated in the function. If not specified, the default probability distribution is the product of a non-informative distribution on the composition matrix, and gamma distributions for the ratio matrix and the data given the model output.
<code>confInt</code>	confidence interval in output; because the distributions may not be symmetrical, standard deviations are not always a useful measure; instead, upper and lower boundaries of the given confidence interval are given. Default is 2/3, i.e there is a probability of 0.66 for a value to be contained within the interval.
<code>export</code>	logical; if TRUE, the function <code>export.bce</code> is called and a list of variables and plots are exported to the specified <code>file</code> .
<code>file</code>	Only if <code>export</code> is TRUE. If not NULL, a character string specifying the file to which objects are saved.

## Details

The function `BCE` searches probability distributions for all elements of a taxonomical composition matrix `X` and a ratio matrix `Rat` for which:

$$X \% * \%Rat \simeq Dat$$

It does this by returning `iter` samples for `X` and `Rat`, organized in three-dimensional arrays. The input data matrix `Dat` and ratio matrix `Rat` should be in the following formats, with the relative concentrations per biomarker organized in columns:

data matrix:

```
marker1  marker2  marker3  marker4
```

sample1	0.14	0.005	0.35	0.033
sample2	0.15	0.004	0.36	0.034
sample3	0.13	0.004	0.31	0.030
sample4	0.13	0.005	0.33	0.031
sample5	0.14	0.008	0.33	0.036
sample6	0.11	0.082	0.34	0.044

and ratio matrix:

	marker1	marker2	marker3	marker4
species1	0.27	0.13	0.35	0.076
species2	0.084	0	0.5	0.24
species3	0.195	0.3	0	0.1
species4	0.06	0	0	0
species5	0	0	0	0
species6	0	0	0	0

### Value

A `bce` (bayesian compositional estimator) object; a list containing 4 elements

<code>Rat</code>	Array with dimension <code>c(nrow(Rat),ncol(Rat), iter)</code> containing the random walk values of the ratio matrix <code>Rat</code> .
<code>X</code>	Array with dimension <code>c(nrow(X),ncol(X),iter)</code> containing the random walk values of the composition matrix <code>X</code> .
<code>logp</code>	vector with length <code>iter</code> containing the random walk values of the (log) posterior probability.
<code>naccepted</code>	integer indicating the number of runs that were accepted.

### Note

Producing sensible output:

Markov Chain Monte Carlo simulations are not as straightforward as one might wish; several preliminary runs might be necessary to determine the desired number of iterations, burn-in length and jump length. For all estimated values of `Rat` and `X`, their trace (evolution of the values over all iterations) has to display random behaviour; no obvious trends should appear. A few parameters can be tuned to obtain such behaviour:

**jump length** The jump length determines how big the jumps are for each step in the random walk. A longer jump length will make you jump around faster in the parameter space, but acceptance of new points can get very low. Smaller jump lengths increase the acceptance rate, but the algorithm will move too slowly, and a lot more runs will be needed to scan the whole parameter space. A good way to find a good jump length, is look at the number of points accepted. If the output is saved under the name `MCMC`, you can find the number of accepted points under `MCMC$naccepted`. It is also given if you run the model with `verbose=TRUE` (default). This value should be somewhere between 5% and 40%. For long runs, 5 % can be acceptable, for short runs, you will prefer a higher acceptance in order to have enough different points. 20% accepted is usually a good number. Do some preliminary runs with

`iter=1000-10000` and tune the jump length parameters `jmpRat` and `jmpX`. You can set different jump lengths for each column of the ratio matrix, or 1 jump length for the whole ratio matrix, and 1 jump length for the composition matrix. Decreasing the jump lengths will generally increase the acceptance rate and vice versa. Also the mixing rate (the speed with which accepted points change their values) will be influenced. You want this mixing rate to be as high as possible, whilst maintaining enough accepted points.

**burninlength** The program uses the solution of lsei using the original ratio matrix as starting values for the MCMC. This might in some cases be far from the optimal solution, and the MCMC algorithm will start with moving towards this optimal solution. This is called a burn-in. When there is a slow mixing rate, this can take a considerable number of cycles. As it can influence the averages and standard deviations, you might want to remove it from the mcmc objects. By defining a burnin length, the first 'burninlength' cycles will not be written to the output. Look at some plots to determine if you need to specify a burnin length.

**iter** the number of iterations: start with 10000 runs or less; check the output and estimate how many runs you will need to get a random pattern in the output.

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#### References

Van den Meersche, K., K. Soetaert and J.J. Middelburg (2008) *A Bayesian compositional estimator for microbial taxonomy based on biomarkers*, Limnology and Oceanography Methods 6, 190-199

#### See Also

[summary.bce](#), [plot.bce](#), [export.bce](#), [pairs.bce](#)

#### Examples

```
##=====
# example using bceInput data
# first try

X <- BCE(bceInput$Rat,bceInput$Dat,relsdRat=.2,relsdDat=.2,
        iter=1000,outputlength=5000,jmpX=.01,jmpRat=.01)

## the number of accepted runs is too low;
## we play around with the jump lengths jmpx and jmprat

X <- BCE(bceInput$Rat,bceInput$Dat,relsdRat=.2,relsdDat=.2,
        iter=1000,outputlength=5000,jmpX=.02,jmpRat=.002)

## we inspect the output:
plot(X)

## For every element of X and Rat, we want to obtain a well-mixed,
## random trace. In this case, mixing is still a little poor.
```

```

## to optimize mixing in the ratio matrix, it is a good idea
## to make the jump length linear to the ratio matrix
## standard deviation (sdrat=.2*rat) :
X <- BCE(bceInput$Rat,bceInput$Dat,relsdRat=.2,relsdDat=.2,
         iter=1000,outputlength=5000,jmpX=.02,
         jmpRat=.2*(.2*bceInput$Rat))
plot(X)

## mixing improved a lot; we repeat the run with more iterations
## to improve the reliability of the results.
## the following run can take a few minutes - so it is toggled off
#X <- BCE(bceInput$Rat,bceInput$Dat,relsdRat=.2,relsdDat=.2,
#         iter=100000,outputlength=5000,jmpX=.02,
#         jmpRat=.2*(.2*bceInput$Rat))
#plot(X)
## you can see in the plots that traces for all elements of Rat and X
## are well-mixed. This run was saved in "bceOutput"

Sum <-summary(bceOutput)

# show results as mean with ranges
print(Sum$meanX)

# plot estimated means and ranges (lbX=lower, ubX=upper bound)
xlim <- range(c(Sum$lbX,Sum$subX))

# first the mean
dotchart(x=t(Sum$meanX),xlim=xlim,
         main="Taxonomic composition",
         sub="using bce",pch=16)

# then ranges
nr <- nrow(Sum$meanX)
nc <- ncol(Sum$meanX)

for (i in 1:nr)
{ip <-(nr-i)*(nc+2)+1
 cc <- ip : (ip+nc-1)
 segments(t(Sum$lbX[i,]),cc,t(Sum$subX[i,]),cc)
}

# show results as pairs plot
pairs(bceOutput,sample=3,main="Station 3")

```

---

bceInput

*ratimatrix and datamatrix for demonstration of BCE().*


---

### Description

The datamatrix contains a set of biomarker measurements for a number of field samples.

The ratiomatrix contains biomarker data of a number of biological taxa. BCE () uses these matrices to estimate the taxonomical composition of the samples based on the provided taxa.

### Usage

```
bceInput
```

### Examples

```
##=====
## Graphical representation of the example input data
palette(rainbow(12, s = 0.6, v = 0.75))

mp      <- apply(bceInput$Rat, MARGIN=2, max)
mp2     <- apply(bceInput$Dat, MARGIN=2, max)
pstars  <- rbind(t(t(bceInput$Rat)/mp), t(t(bceInput$Dat)/mp2))

stars(pstars, len = 0.9, key.loc = c(7.2, -2), scale=FALSE,
      ncol=5, ylim=c(0,3), main = "bce Input: species + field samples",
      draw.segments = TRUE, flip.labels=FALSE)
```

---

```
bceOutput
```

*bce output generated by running the bceInput example*

---

### Description

Result generated by running BCE using data bceInput as input.

the run was initiated with the following command:

```
bceOutput <- BCE(bceInput$Rat, bceInput$Dat, relsdRat=.2, relsdDat=.2,
  iter=100000, outputlength=5000, jmpX=.02, jmpRat=.2*(.2*bceInput$Rat))
```

this run took several minutes.

### Usage

```
bceOutput
```

### Examples

```
summary(bceOutput)$meanX
```

---

`export.bce`*export BCE*

---

## Description

export function: writes a BCE-object and its summary statistics to a series of files.

## Usage

```
export.bce(x, file="BCE", input.list=NULL, ...)
```

## Arguments

<code>x</code>	a bce object, output of the function <code>bce()</code> .
<code>file</code>	file to which the bce object is written.
<code>input.list</code>	a list of the arguments in <code>bce()</code> can be provided and saved as well.
<code>...</code>	additional arguments.

## Details

The bce object is saved ([save](#)) to the specified file. For people not familiar to R, it can be more 'user-friendly' to export summary results to comma delimited textfiles, that can be easily imported into a spreadsheet program. The function [summary.bce](#) is called to calculate summary statistics of a BCE object; These are then written to a series of .csv files with a name that combines the specified filename and a string indicating the content of the .csv files. Traces and marginal probabilities of all estimated values are plotted and saved in .png files. These traces should be inspected carefully before accepting any results (see also [plot.bce](#)).

## Author(s)

Karel Van den Meersche

## See Also

[BCE](#), [summary.bce](#), [plot.bce](#), [pairs.bce](#)

## Examples

```
## Not run: export.bce(bceOutput, file="bceOutput")
```

---

pairs.bce	<i>A pairs plot of a BCE</i>
-----------	------------------------------

---

## Description

produces a pairs plots of the random walks of the BCE.

## Usage

```
pairs.bce(x, sample=1, gap=0, upper.panel = NA,  
          diag.panel = NA, ...)
```

## Arguments

x	either a bce object or the random walk values ( $\bar{x}$ ) of the composition matrix.
sample	the sample number for which the pairs plot is to be drawn.
gap	Distance between subplots, in margin lines - a <code>pairs</code> parameter.
upper.panel	panel function to be used above the diagonal - the default writes the correlations.
diag.panel	panel function to be used on the diagonal - the default plots a histogram.
...	any other parameters passed to function <code>pairs</code> .

## Author(s)

Karline Soetaert

## See Also

[BCE](#), [summary.bce](#), [plot.bce](#), [export.bce](#)

## Examples

```
# bceOutput is an example output based on bceInput  
pairs(bceOutput, sample=2, main="Station 2")
```

---

`plot.bce`*plot BCE*

---

## Description

produces summary plots of the random walks of the BCE; these are intended for inspection only.

## Usage

```
plot.bce(x, ...)
```

## Arguments

<code>x</code>	bce object.
<code>...</code>	additional arguments.

## Details

Calling the plot-function with a bce-object as argument, will produce a series of plots with the random walks of each variable. The layout of these plots is kept very sober, as they are primarily intended for inspection of the random walk (see [BCE](#)). Users are free to write their own publication quality plots. Click or hit Enter to see the next plot, hit Esc to stop seeing new plots.

## Author(s)

Karel Van den Meersche

## See Also

[BCE](#), [summary.bce](#), [export.bce](#), [pairs.bce](#)

## Examples

```
# bceOutput is an example output based on bceInput  
  
plot(bceOutput)
```

---

rescaleRows	<i>rescale rows</i>
-------------	---------------------

---

**Description**

returns a row-rescaled matrix (`rowSums(.) == 1`).

**Usage**

```
rescaleRows(A, columns=1:ncol(A))
```

**Arguments**

A	matrix or dataframe to be row-rescaled: <code>rowSums(rescaleRows(A)) == 1</code> .
columns	vector containing indices of the columns that should be included in the normalisation.

**Value**

A	row-rescaled matrix or partially row-rescaled matrix.
---	---

**Author(s)**

Karel Van den Meersche

---

summary.bce	<i>summary BCE</i>
-------------	--------------------

---

**Description**

basic statistics of a bce object

**Usage**

```
summary.bce(object, confInt=2/3, ...)
```

**Arguments**

object	a bce-object, output of the function <code>bce()</code> .
confInt	confidence interval of values of composition matrix and ratio matrix.
...	additional arguments affecting the summary produced.

**Value**

a list containing:

<code>firstX</code>	X determined through least squares regression from the initial ratio matrix and the data matrix.
<code>bestRat</code>	Ratio matrix for which the posterior probability is maximal.
<code>bestX</code>	Composition matrix for which the posterior probability is maximal.
<code>bestp</code>	Maximal posterior probability.
<code>bestDat</code>	Product of <code>bestRat</code> and <code>bestX</code> .
<code>meanRat</code>	Means of the elements of the ratio matrix.
<code>sdRat</code>	Standard deviation of the elements of the ratio matrix.
<code>lbRat</code>	Lower boundary of the confidence interval of the elements of the ratio matrix.
<code>ubRat</code>	Upper boundary of the confidence interval of the elements of the ratio matrix.
<code>covRat</code>	Covariance matrix of the elements of the ratio matrix.
<code>meanX</code>	Means of the elements of the composition matrix.
<code>sdX</code>	Standard deviation of the elements of the composition matrix.
<code>lbX</code>	Lower boundary of the confidence interval of the elements of the composition matrix.
<code>ubX</code>	Upper boundary of the confidence interval of the elements of the composition matrix.
<code>covX</code>	Covariance matrix of the elements of the composition matrix.

**Author(s)**

Karel Van den Meersche

**See Also**

[BCE](#), [plot.bce](#), [export.bce](#), [pairs.bce](#)

**Examples**

```
# bceOutput is an example output based on bceInput
summary(bceOutput)
```

---

 tlsce

*Total Least Squares Composition Estimator*


---

### Description

estimates a matrix X for which:

$$(A + \epsilon_A)X = B + \epsilon_B$$

minimize  $\sum \epsilon_A^2 + \epsilon_B^2$

$$\sum X_i = 1 \forall i$$

$$X > 0$$

the elements of  $\epsilon_A$  are NULL if the corresponding elements of A are NULL. A typically contains biomarker concentrations for several taxonomic groups, and B field measurements of the same biomarkers. X is then an estimate of the taxonomic composition of the field sample.

### Usage

```
tlsce(A, B, Wa=NULL, optimizationfunction="nlminb",
      A_init=A, Xratios=TRUE, ...)
```

### Arguments

A	a matrix or data frame. If A contains biomarker data for taxonomic groups, the biomarkers have to be organized per row, and the taxonomic groups per column.
B	a matrix or data frame. If B contains biomarker field data, the biomarkers have to be organized per row, and the samples per column.
Wa	weighting of A, a matrix with the same dimensions of A. If Wa=NULL, Wa defaults to 1. This parameter can be used to give more importance to elements of A or A in total compared to B. Weighting of B is not possible. the weights are implemented as proportional to $1/s$ (as opposed to $1/s^2$ ) with s the standard deviation of the error term.
optimizationfunction	the function used for the optimization of A (one of "nlminb", "optim", "constrOptim").
A_init	a matrix with the same structure as A. a general, non-linear optimization routine (default nlminb) is used to minimize the sum of squared residuals of A versus the fitted matrix A_fit (see value). This optimization routine requires a set of starting values, by default the non-zero elements of A. This provides a good fit, but when in doubt about the convergence of the algorithm, one can provide different starting values for the optimization routine in A_init.
Xratios	TRUE or FALSE: are the colSums of the matrix X equal to 1? This is for example the case in a compositional matrix.
...	Arguments to be passed to the optimization function in use.

**Details**

instead of a linear least squares regression, in which the elements of A would be fixed, the function `tlsce` includes the non-zero elements of A in the least squares regression. This is similar to other total least squares regression methods, with the main difference that only non-zero elements of A contain an error term.

**Value**

A list with the following elements:

<code>X</code>	Array with dimension <code>c(ncol(A),ncol(B), iter)</code> containing the species composition of each sample
<code>A_fit</code>	Array with same dimension as A, containing the best-fit values of the input biomarker data per taxonomic group
<code>B_fit</code>	Array with same dimension as B, containing the biomarker field data, corresponding to Afit
<code>solutionNorms</code>	a vector of 3 values: the value of the minimised quadratic function at the solution, in this case $\sum (Afit - A) * Wa)^2 + (Bfit$ and the shares of this value attributed to A and to B
<code>convergence</code>	An integer code. '0' indicates successful convergence.

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**References**

Van den Meersche, K., K. Soetaert and J.J. Middelburg (2008) *A Bayesian compositional estimator for microbial taxonomy based on biomarkers*, Limnology and Oceanography Methods 6, 190-199

**See Also**

[BCE](#)

**Examples**

```
A <- t(bceInput$Rat)
B <- t(bceInput$Dat)
tlsce(A,B)
## weighting Wa inversely proportional to A
tlsce(A,B,Wa=1/A)
```

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