

Package: CoDaLoMic (via r-universe)

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Type Package

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Description Implementation of models to analyse compositional microbiome time series taking into account the interaction between groups of bacteria. The models implemented are described in Creus-Martí et al (2018, ISBN:978-84-09-07541-6), Creus-Martí et al (2021) <[doi:10.1155/2021/9951817](https://doi.org/10.1155/2021/9951817)> and Creus-Martí et al (2022) <[doi:10.1155/2022/4907527](https://doi.org/10.1155/2022/4907527)>.

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Description

This package contains functions to model compositional and longitudinal microbiome datasets. This package contains the functions needed to execute the models published in the articles:

- Creus-Martí, I., Moya, A., Santonja, F. J. (2018), A Statistical Model with a Lotka-Volterra Structure for Microbiota Data, Lucas Jodar, Juan Carlos Cortes and Luis Acedo, Modelling for engineering and human behavior 2018, Instituto Universitario de Matematica Multidisciplinar, ISBN: 978-84-09-07541-6.
- Creus-Martí, I., Moya, A., Santonja, F. J. (2021). A Dirichlet autoregressive model for the analysis of microbiota time-series data. Complexity, 2021, 1-16.
- Creus-Martí, I., Moya, A., Santonja, F. J. (2022). Bayesian hierarchical compositional models for analysing longitudinal abundance data from microbiome studies. Complexity, 2022.

In addition, the package contains one real dataset extracted from:

- Marín-Miret, J., Pérez-Cobas, A. E., Domínguez-Santos, R., Pérez-Rocher, B., Latorre, A., & Moya, A. (2024). Adaptability of the gut microbiota of the German cockroach *Blattella germanica* to a periodic antibiotic treatment. Microbiological Research, 287, 127863.

Details

We refer to the model described in Creus-Martí (2018) as Dirich-gLV, we refer to the model described in Creus-Martí (2021) as FBM and we refer to the model described in Creus-Martí (2022) as BPBM.

Access to Additional Files

This package includes files in the directory 'inst/extdata'. Users can access these files using 'system.file()'. The following files are available:

- README.pdf, README.Rmd, README.R: Basic instructions for using the package.
- 1-s2.0-S0944501324002647-mm6.xlsx: Original cockroach dataset extracted from Marín-Miret et al (2024).
- Simulated.R: Code use to obtain the Simulated dataset.
- cockroach.R: Code use to obtain the cockroach dataset.

To access these files, use: `base::system.file("extdata", "filename", package = "CoDaLoMic")`

For instance: `base::system.file("extdata", "README.pdf", package = "CoDaLoMic")`

On Windows, the PDF can be opened as follows: `base::shell.exec(system.file("extdata", "README.pdf", package = "CoDaLoMic"))`

Author(s)

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 B1MODImatrizP

Ridge regression matrix

Description

Defining the part of the ridge regression matrix that carries the information of the bacteria especieII.

Usage

```
B1MODImatrizP(Tt, especieII, especie, E, EspecieMaxima)
```

Arguments

Tt	Number of time points available
especieII	Number. The number of the row in which the bacteria that we want to use is placed in the matrix especie.
especie	Matrix that contains at row i the bacterial taxa of bacteria i at all time points.
E	Number of bacteria available
EspecieMaxima	Row in which the bacteria chosen as reference is in especie. This is the bacteria that is going to be at the denominator of the balance and at the denominator of the alr transformation.

Value

Returns a matrix. The first column contain the number 1 repeated Tt times. The second column contains the alr transformation of the especieII in all time points. The third column contains the balance (whose numerator has all the bacteria except especieII and EspecieMaxima and the denominator contains the EspecieMaxima) in all time points.

Examples

```
Tt=2
especie1=cbind(c(0.5,0.3,0.2), c(0.1,0.3,0.6))
especieII=1
E=3
EspecieMaxima=3

B1MODImatrizP(Tt, especieII,especie1, E, EspecieMaxima)
```

B1MODImodel

*Obtaining the regression value of the FBM***Description**

This function calculates the value of the FBM regression, defined by:

$$\mu_{it} = a_{i1} + a_{i2} \cdot \text{alr}(x_{i,(t-1)}) + a_{i3} \cdot \text{Balance}(x_{i,(t-1)}) \text{ for } i = 1, \dots, D-1 \text{ where } D \text{ is the number of bacteria}$$

Usage

```
B1MODImodel(A, especie, E, EspecieMaxima, Tt)
```

Arguments

A	Matrix of dimensions (E-1)x3 that contains all the parameters of the model except tau
especie	Matrix that contains at row i the bacterial taxa of bacteria i at all time points.
E	Number of bacteria available
EspecieMaxima	Row in which the bacteria chosen as reference is in especie. This bacteria is used as reference in the alr transformation that the model does and it is placed at the denominator of the balance)
Tt	Number of time points available.

Value

Returns a matrix. The row i contains the regression values of the bacteria i at all time points.

References

Creus-Martí, I., Moya, A., Santonja, F. J. (2021). A Dirichlet autoregressive model for the analysis of microbiota time-series data. *Complexity*, 2021, 1-16.

Examples

```
df<-data.frame(cbind(c(0.1,0.1,0.8),c(0.2,0.1,0.7)))
E=3
EspecieMaxima=3
set.seed(724)
A=matrix(c(-2:3),2,3)
Tt=2

B1MODImodel(A,df, E, EspecieMaxima,Tt)
```

Balance *Calculating the balance of the FBM model*

Description

Defining a balance where we compare all the bacteria (except the one chosen as reference and the especieI) with the one chosen as reference.

Usage

```
Balance(A, especieI, especie, E, EspecieMaxima)
```

Arguments

A	Number of time points for which we calculate the balance
especieI	Number. The bacteria that we do not include in the balance. We must write the number of the row in which the bacteria is placed in the matrix especie.
especie	Matrix that contains at row i the bacterial taxa of bacteria i at all time points.
E	Number of bacteria available
EspecieMaxima	Row in which the bacteria chosen as reference is in especie. This bacteria is used as reference in the alr transformation that the model does and it is placed at the denominator of the balance)

Value

Returns a vector with the value of the balance for all the time points indicated.

Examples

```
Balance(2,2,cbind(c(0.1,0.1,0.8),c(0.2,0.1,0.7)),3,3)
```

BPBM_Matrix *Obtains the matrix of covariates of the BPBM*

Description

This function writes the matrix of covariates of the BPBM.

Usage

```
BPBM_Matrix(rows.position, PB, Tt)
```

Arguments

rows.position	Vector. Vector with the number of the rows where the SPBal are in the matrix PB. We write first the row in which the balance with higher variance is placed, then the row in which the balance with second higher variance is placed...
PB	Matrix. Each line os the matrix PB contains the values of one principal balance at all time points.
Tt	Number of time points available.

Details

In an example with two SPBal and three time points, the covariates are written in the following order:

$$\begin{array}{ccc} 1 & 1 & 1 \\ SPBal_{1,t-1} & SPBal_{1,t-2} & SPBal_{1,t-3} \\ SPBal_{2,t-1} & SPBal_{2,t-2} & SPBal_{2,t-3} \end{array}$$

Value

Returns a matrix with the covariates of the model.

References

Creus-Martí, I., Moya, A., Santonja, F. J. (2022). Bayesian hierarchical compositional models for analysing longitudinal abundance data from microbiome studies. *Complexity*, 2022.

Examples

```
matt=matrix(c(1:12),3,4)
rows.position=c(2,3)
BPBM_Matrix(rows.position,matt,4)
```

cockroach

cockroach dataset

Description

Gut microbiome dataset of a *Blattella germanica* cockroach treated by kanamycin during three periods of time (days: 1–10, 36–45, 71–80). The data is extracted from Marín-Miret et al (2024), more specifically, the data is the information of the K3 cockroach in the article. The dataset contains 105 time points and 210 genera.

Usage

```
data(cockroach)
```

Format

A data frame with 105 rows and 211 columns.

References

Marín-Miret, J., Pérez-Cobas, A. E., Domínguez-Santos, R., Pérez-Rocher, B., Latorre, A., & Moya, A. (2024). Adaptability of the gut microbiota of the German cockroach *Blattella germanica* to a periodic antibiotic treatment. *Microbiological Research*, 287, 127863.

Estimate_Param_EstParmFunc

Estimating Parameters of EstParmFunc

Description

This function calculates the estimated parameters of the Dirich-gLV model.

Usage

```
Estimate_Param_EstParmFunc(Iter.EstParmFunc, paramini, especie, seed = NULL)
```

Arguments

<code>Iter.EstParmFunc</code>	Number. Number of iterations.
<code>paramini</code>	Initial values of the parameters. Vector equal to <code>c(tau.ini, as.vector(pam.ini))</code> where:
<code>especie</code>	Matrix that contains at row <i>i</i> the bacterial taxa of bacteria <i>i</i> at all time points. The bacteria placed in the last row of the matrix will be used as reference in the alr transformation.
<code>seed</code>	Number. Set a seed. Default <code>seed=NULL</code> . <ul style="list-style-type: none"> • <code>pam.ini</code> Matrix. Each row has the parameters of each bacteria, following the same structure than <code>pam</code> in <code>EstParmFunc</code> • <code>tau.ini</code> Number. Initial value of the tau parameter in the model

Details

Maximum likelihood estimation is used. This function makes an iterative process, it obtains the value of the parameter that maximize the Dirichlet loglikelihood (defined in `EstParmFunc`) using the Nelder-Mead method and some initial parameters. Then it uses this value as initial parameters and repeats the process `Iter.EstParmFunc` times.

Value

Returns a list with:

- All.iter: Matrix. Each row has the parameters obtained in each iteration. The parameters are in the columns written in the same order that they are written in paramini. In this matrix we must observe that in the last iterations the values has really similar or equal values, it not, we need to increase the value of Iter.EstParmFunc.
- Param.Estimates: The estimated parameters. The parameters are in the columns written in the same order that they are written in paramini.

References

Creus-Martí, I. and Moya, A. and Santonja, F. J. (2018). A Statistical Model with a Lotka-Volterra Structure for Microbiota Data. Lucas Jodar, Juan Carlos Cortes and Luis Acedo, Modelling for engineering and human behavior 2018, Instituto Universitario de Matematica Multidisciplinar. ISBN: 978-84-09-07541-6

Examples

```
especie=cbind(c(0.5,0.3,0.2),c(0.1,0.3,0.6))
paramini=c(100,2,3,4,5,6,7)
Estimate_Param_EstParmFunc(5, paramini , especie,714)
```

Estimate_Param_FBM *Estimating Parameters of EstParmFunc_FBM*

Description

This function estimates the parameters of the FBM model.

Usage

```
Estimate_Param_FBM(
  tau,
  ridge.final,
  Iter.EstParmFunc = 80,
  especie,
  EspecieMaxima,
  Tt,
  E,
  seed = NULL
)
```

Arguments

<code>tau</code>	Number. Value of the tau parameter.
<code>ridge.final</code>	Object of class "ridgelm". Values obtained with the ridge regression.
<code>Iter.EstParmFunc</code>	Number. Number of iterations. Default: 80 iterations.
<code>especie</code>	Matrix that contains at row <i>i</i> the bacterial taxa of bacteria <i>i</i> at all time points. The bacteria placed in the last row of the matrix will be used as reference in the alr transformation and will be at the denominator of the balance.
<code>EspecieMaxima</code>	Row in which the bacteria chosen as reference is in <code>especie</code> . This is the bacteria that is going to be at the denominator of the balance and in the denominator of the alr transformation. As a result, in this function, <code>EspecieMaxima</code> must be equal to <code>E</code> .
<code>Tt</code>	Number of time points available
<code>E</code>	Number. Number of bacteria available.
<code>seed</code>	Number. Set a seed. Default <code>seed=NULL</code> .

Details

Maximum likelihood estimation is used. This function makes an iterative process, for a given value of tau, it obtains the value of the rest of the parameters that maximize the dirichlet loglikelihood (defined in `EstParmFunc_FBM`) using the Nelder-Mead method and the values obtained in the ridge regression as initial parameters. Then it uses the values obtained as initial parameters and repeats the process `Iter.EstParmFunc` times.

The regression of this model is defined by

$$\mu_{it} = a_{i1} + a_{i2} \cdot \text{alr}(x_{i,(t-1)}) + a_{i3} \cdot \text{Balance}(x_{i,(t-1)}) \text{ for } i = 1, \dots, D-1 \text{ where } D \text{ is the number of bacteria}$$

Value

Returns a list with:

- `All.iter`: Matrix. Each row has the parameters obtained in each iteration. The parameters are in the columns written in following order: `a11,a12,a13, a21, a22,a23, ...a(D-1)1,a(D-1)2,a(D-1)3,tau`. Where `D` is the number of bacterial species present in the matrix `especie`. In this matrix we must observe that in the last iterations the values has really similar or equal values, if not, we need to increase the value of `Iter.EstParmFunc`.
- `Param.Estimates`: Vector with the estimated parameters, in the following order: `a11,a12,a13, a21, a22,a23, ...a(D-1)1,a(D-1)2,a(D-1)3,tau`. Where `D` is the number of bacterial species present in the matrix `especie`.
- `AIC Number`: Value of the AIC.

References

Creus-Martí, I., Moya, A., Santonja, F. J. (2021). A Dirichlet autoregressive model for the analysis of microbiota time-series data. *Complexity*, 2021, 1-16.

Examples

```

set.seed(123)
especie=t(gtools::rdirichlet(5,c(1,3,1)))
Tt=5
E=3
EspecieMaxima=3
ridge.final=ridgeregression(Tt,especie, E, EspecieMaxima)
tau=20
Iter.EstParmFunc=40

Estimate_Param_FBM(tau,ridge.final,Iter.EstParmFunc, especie,EspecieMaxima,Tt,E, 714)

```

 Estimating_BPBM

Estimating BPBM

Description

The estimation of the BPBM model is carried out using MCMC. To execute this function it is necessary to have the program Just Another Gibbs Sampler (JAGS) (Plummer, 2003) program installed.

Usage

```

Estimating_BPBM(
  especie,
  Tt,
  E,
  MatrizPBmodelo,
  nn.chain = 3,
  nn.burnin = 5000,
  nn.sample = 20000,
  nn.thin = 10,
  seed = NULL
)

```

Arguments

especie Matrix that contains at row i the bacterial taxa of bacteria i at all time points.

Tt Number of time points available.

E Number of bacteria in the dataset.

MatrizPBmodelo Matrix with the covariates of the model. In an example with two SPBal and three time points, the covariates are written in the following order:

$$\begin{array}{ccc}
 & 1 & 1 & 1 \\
 SPBal_{1,t-1} & SPBal_{1,t-2} & SPBal_{1,t-3} \\
 SPBal_{2,t-1} & SPBal_{2,t-2} & SPBal_{2,t-3}
 \end{array}$$

<code>nn.chain</code>	the number of chains to use with the simulation. Default is 3, minimum2.
<code>nn.burnin</code>	the number of burnin iterations. Default is 5000.
<code>nn.sample</code>	the number of iterations to take. Default: 20000. The markov chain will have ("sample"- "burnin")/"thin" iterations.
<code>nn.thin</code>	the thinning interval to be used. Default: 10.
<code>seed</code>	Number. Set a seed. Default seed=NULL.

Value

Returns a list with:

- List with:
 - `R2jagsOutput`: R2jags object with the information of the estimation.
 - `SamplesAllChains`: Matrix. Matrix that has the iterations of all the Markov chains joined.

References

- Creus-Martí, I., Moya, A., Santonja, F. J. (2022). Bayesian hierarchical compositional models for analysing longitudinal abundance data from microbiome studies. *Complexity*, 2022.
- Plummer, M. (2003, March). JAGS: A program for analysis of Bayesian graphical models using Gibbs sampling. In *Proceedings of the 3rd international workshop on distributed statistical computing* (Vol. 124, No. 125.10, pp. 1-10).

Examples

```
set.seed(314)
especie=t(gtools::rdirichlet(n=6, c(6,6,1,6,6)))
E=5
Tt=6
MatrizPBmodelo=rbind(c(1,1,1,1,1,1),c(-0.3,0.4,0.3,-0.7,-0.4,-0.6),c(0.3,0.5,-0.3,0.1,0.4,0.1))
```

```
Estimating_BPBM(especie,
                Tt,
                E,
                MatrizPBmodelo,
                nn.chain=3,
                nn.burnin=1000,
                nn.sample=2000,
                nn.thin=10,
                714)
```

 EstParmFunc

Writing the loglikelihood of the dirichlet

Description

This function calculates the loglikelihood of the dirichlet for the Dirich-gLV model.

Usage

```
EstParmFunc(parms.vector, especie)
```

Arguments

`parms.vector` Vector equal to `c(tau, as.vector(pam))` where:

- `pam`: Matrix. Each row has the parameters of each bacteria. Following our example, `pam` has the parameters placed as follows:

$$\begin{array}{ccc} r1 & a11 & a12 \\ r2 & a21 & a22 \end{array}$$

- `tau`: Number. Value of the tau parameter in the model

`especie` Matrix that contains at row `i` the bacterial taxa of bacteria `i` at all time points . The bacteria placed in the last row of this matrix is the one used as reference in the alr transformation that the model apply

Details

In an example with three bacteria, the regression of this model is defined by

$$r_1 \cdot \log(x_1(t)/x_3(t)) + \log(x_1(t)/x_3(t)) \cdot [a_{11} \cdot \log(x_1(t)/x_3(t))(t) + a_{12} \cdot \log(x_2(t)/x_3(t))]$$

$$r_2 \cdot \log(x_2(t)/x_3(t)) + \log(x_2(t)/x_3(t)) \cdot [a_{21} \cdot \log(x_1(t)/x_3(t))(t) + a_{22} \cdot \log(x_2(t)/x_3(t))]$$

Value

Returns a number with the value of the dirichlet loglikelihood.

References

Creus-Martí, I. and Moya, A. and Santonja, F. J. (2018). A Statistical Model with a Lotka-Volterra Structure for Microbiota Data. Lucas Jodar, Juan Carlos Cortes and Luis Acedo, Modelling or engineering and human behavior 2018, Instituto Universitario de Matematica Multidisciplinar. ISBN: 978-84-09-07541-6

Examples

```

especie1=cbind(c(0.5,0.3,0.2), c(0.1,0.3,0.6))
tau1=0.4
parms1= cbind(c(0.1,0.2),c(-0.2,0.1),c(0.3,0.2))
parms11=c(tau1,as.vector( parms1))

EstParmFunc(parms11,especie1)

```

EstParmFunc_FBM

Writing the loglikelihood of the dirichlet

Description

This function calculates the loglikelihood of the dirichlet for the FBM model.

Usage

```
EstParmFunc_FBM(param, especie, E, EspecieMaxima, Tt, especiemodi)
```

Arguments

param	Vector with the parameters in the following order: a11,a12,a13, a21, a22,a23, ...a(D-1)1,a(D-1)2,a(D-1)3,tau. Where D is the number of bacterial species present in the matrix especie.
especie	Matrix that contains at row i the bacterial taxa of bacteria i at all time points.
E	Number of bacteria available
EspecieMaxima	Row in which the bacterial with maximum mean abundance is in especie.This bacteria is used as reference in the alr transformation that the model does and it is placed at the denominator of the balance)
Tt	Number of bacteria available
especiemodi	Matrix that contains at row i the bacterial taxa of bacteria i at time points t=2,...,Tt. The bacteria are placed in the same order than in especie.

Details

The regression of this model is defined by

$$\mu_{it} = a_{i1} + a_{i2} \cdot \text{alr}(x_{i,(t-1)}) + a_{i3} \cdot \text{Balance}(x_{i,(t-1)}) \text{ for } i = 1, \dots, D-1 \text{ where } D \text{ is the number of bacteria}$$

Value

Returns a number with the value of the dirichlet loglikelihood.

References

Creus-Martí, I., Moya, A., Santonja, F. J. (2021). A Dirichlet autoregressive model for the analysis of microbiota time-series data. *Complexity*, 2021, 1-16.

Examples

```
especie1=cbind(c(0.5,0.3,0.2), c(0.1,0.3,0.6))
especiemodi=especie1[,-1]
tau1=0.4
parms1= cbind(c(0.1,0.2),c(-0.2,0.1),c(0.3,0.2))
parms11=c(as.vector( t(parms1)),tau1)

EstParmFunc_FBM(parms11,especie1,3 ,3 , 2,especiemodi)
```

ExpectedValuess_BPBM *Obtainig the value of the dirichlet parameters, the expected value and the variance.*

Description

This function calculates the value of the dirichlet parameters, the expected value and the variance for the BPBM model.

Usage

```
ExpectedValuess_BPBM(Estimated.Param, MatrizPBmodelo, E, Tt)
```

Arguments

Estimated.Param	Vector with the estimate parameters. Column "mean" of the output of "StudyingParam" function.
MatrizPBmodelo	Matrix. Output of "ObtainingValueSPBal" called "MatrixSPBal".
E	Number of bacteria available.
Tt	Number of time points available.

Details

The regression of this model is defined by:

$$\mu_{it} = a_{i0} + a_{i1} \cdot \text{SPBal}_{1,t-1} + \dots + a_{iM} \cdot \text{SPBal}_{M,t-1}$$

Value

Returns a list with:

- **Dirichlet.Param:** Matrix. Matrix that contains at row *i* the dirichlet parameter of the bacteria *i* at all time points.
- **Expected.Value:** Matrix. Matrix that contains at row *i* the expected value of the bacteria *i* at all time points. The bacterias are placed at the same orden than in especies.
- **Variance.Value:** Matrix. Matrix that contains at row *i* the variance of the bacteria *i* at all time points. The bacterias are placed at the same orden than in especies.

References

Creus-Martí, I., Moya, A., Santonja, F. J. (2022). Bayesian hierarchical compositional models for analysing longitudinal abundance data from microbiome studies. *Complexity*, 2022.

Examples

```
Tt=3
E=3
Estimated.Param=c(0.1 ,0.4, 0.7, 0.2 ,0.5, 0.8 ,0.3, 0.6, 0.9,
                  0.1, 0.4 ,0.7, 0.2, 0.5, 0.8, 0.3 ,0.6, 0.9)
MatrizPBmodelo=rbind(c(1,1,1),c(0.3,0.6,-0.1),c(0.2,-0.4,0.3))
ExpectedValues_BPBM(Estimated.Param,MatrizPBmodelo,E,Tt)
```

ExpectedValues_EstParmFunc_FBM

Obtainig the value of the dirichlet parameters, the expected value and the variance.

Description

This function calculates the value of the dirichlet parameters, the expected value and the variance for the FBM model.

Usage

```
ExpectedValues_EstParmFunc_FBM(
  paramEstimadosFinal,
  especie,
  E,
  EspecieMaxima,
  Tt
)
```


Arguments

paramEstimadosFinal	The estimate parameters, in the following order: $a_{11}, a_{12}, a_{13}, a_{21}, a_{22}, a_{23}, \dots, a_{(D-1)1}, a_{(D-1)2}, a_{(D-1)3}, \tau$. Where D is the number of bacterial species present in the matrix <code>especie</code> .
especie	Matrix that contains at row i the bacterial taxa of bacteria i at all time points.
E	Number of bacteria available.
EspecieMaxima	Row in which the bacteria chosen as reference is in <code>especie</code> . This bacteria is used as reference in the <code>alr</code> transformation that the model does and it is placed at the denominator of the balance).
Tt	Number of time points available.

Details

The regression of this model is defined by

$$\mu_{it} = a_{i1} + a_{i2} \cdot \text{alr}(x_{i,(t-1)}) + a_{i3} \cdot \text{Balance}(x_{i,(t-1)}) \text{ for } i = 1, \dots, D-1 \text{ where } D \text{ is the number of bacteria}$$

Value

Returns a list with:

- `Dirichlet.Param`: Matrix. Matrix that contains at row i the dirichlet parameter of the bacteria i at all time points.
- `Expected.Value`: Matrix. Matrix that contains at row i the expected value of the bacteria i at all time points. The bacterias are placed at the same orden than in `especies`.
- `Variance.Value`: Matrix. Matrix that contains at row i the variance of the bacteria i at all time points. The bacterias are placed at the same orden than in `especies`.

References

Creus-Martí, I., Moya, A., Santonja, F. J. (2021). A Dirichlet autoregressive model for the analysis of microbiota time-series data. *Complexity*, 2021, 1-16.

Examples

```
set.seed(123)
especie=t(gtools::rdirichlet(2,c(1,1,3)))
Tt=2
E=3
tau=5
EspecieMaxima=3
Iter.EstParmFunc=5
parms11=c(0.1,0.2,0.3,0.4,0.5,0.6,tau)

ExpectedValues_EstParmFunc_FBM(parms11 , especie,E,EspecieMaxima,Tt)
```

ExpectedValue_EstParmFunc

Obtaining the value of the Dirichlet parameters, the expected value and the variance.

Description

This function calculates the value of the Dirichlet parameters, the expected value and the variance for the Dirich-gLV model.

Usage

```
ExpectedValue_EstParmFunc(Param.Estimates, especie)
```

Arguments

Param.Estimates

Vector with the estimated parameters. This value is the output of the Estimate_Param_EstParmFunc function.

especie

Matrix that contains at row i the bacterial taxa of bacteria i at all time points. The bacteria placed in the last row of this matrix is the one used as reference in the alr transformation that the model applies.

Value

Returns a list with:

- Dirichlet.Param: Matrix. Matrix that contains at row i the Dirichlet parameter of the bacteria i at all time points.
- Expected.Value: Matrix. Matrix that contains at row i the expected value of the bacteria i at all time points. The bacterias are placed at the same orden than in especies.
- Variance.Value: Matrix. Matrix that contains at row i the variance of the bacteria i at all time points. The bacterias are placed at the same orden than in especies.

References

Creus-Martí, I. and Moya, A. and Santonja, F. J. (2018). A Statistical Model with a Lotka-Volterra Structure for Microbiota Data. Lucas Jodar, Juan Carlos Cortes and Luis Acedo, Modelling or engineering and human behavior 2018, Instituto Universitario de Matematica Multidisciplinar. ISBN: 978-84-09-07541-6

Examples

```
especie1=cbind(c(0.5,0.3,0.2), c(0.1,0.3,0.6))
tau1=0.4
parms1= cbind(c(0.1,0.2),c(-0.2,0.1),c(0.3,0.2))
```

```
parms11=c(tau1,as.vector( parms1))
ExpectedValue_EstParmFunc(parms11,especie1)
```

FromVectorToMatrix_BPBM

Writing the parameters in the matrix form required in BPBM model

Description

StudyingParam returns a matrix where the value of the parameters is in the column "mean". This function inputs this columns and outputs the parameters in the matrix form required by the BPBM model.

Usage

```
FromVectorToMatrix_BPBM(param, MatrizPBmodelo, E)
```

Arguments

param Vector. Column "mean" of the output of "StudyingParam" function.

MatrizPBmodelo Matrix with the covariates of the model. In an example with two SPBal and three time points, the covariates are written in the following order:

	1	1	1
	<i>SPBal</i> _{1,t-1}	<i>SPBal</i> _{1,t-2}	<i>SPBal</i> _{1,t-3}
	<i>SPBal</i> _{2,t-1}	<i>SPBal</i> _{2,t-2}	<i>SPBal</i> _{2,t-3}

E Number of bacteria in the dataset.

Value

Returns a matrix with the parameters in the order required by the BPBM model.

References

Creus-Martí, I., Moya, A., Santonja, F. J. (2022). Bayesian hierarchical compositional models for analysing longitudinal abundance data from microbiome studies. *Complexity*, 2022.

Examples

```
set.seed(314)
especie=t(gtools::rdirichlet(n=6, c(6,6,1,6,6)))
E=5
Tt=6
MatrizPBmodelo=rbind(c(1,1,1,1,1),
                     c(-0.3,0.4,0.3,-0.7,-0.4,-0.6),
                     c(0.3,0.5,-0.3,0.1,0.4,0.1))
```

```

est=Estimating_BPBM(especie,
                    Tt,
                    E,
                    MatrizPBmodelo,
                    nn.chain=3,
                    nn.burnin=1000,
                    nn.sample=5000,
                    nn.thin=10)

mm=StudyingParam(est$R2jagsOutput$BUGSoutput$summary, est$SamplesAllChains)
FromVectorToMatrix_BPBM(mm$Param.Summary[, "mean"], MatrizPBmodelo, 5)

```

FVectorPBmodeloPredi *Obtaining a vector with the covariates of the prediction*

Description

Calculates a vector with the covariates of the BPBM model in one time point.

Usage

```
FVectorPBmodeloPredi(NumSPBal, DemSPBal, v, MatrizPBmodelo)
```

Arguments

NumSPBal	List. The component i of the list has the number of the row of the matrix especie where the bacteria in the numerator of the principal balance i are placed.
DemSPBal	List. The component i of the list has the number of the row of the matrix especie where the bacteria in the denominator of the principal balance i are placed.
v	Vector. Vector with a coda composition. The bacteria are in the same order than the matrix especie
MatrizPBmodelo	the matrix that contains the covariates of the model. The first line is equal to 1 for all columns. The other rows contain the value of one SPBal at all time points. The selected principal balance of the row $i+1$ has at its numerator the bacteria placed in the rows NumSPBal[[i]] of the "especie". The selected principal balance of the row $i+1$ has at its denominator the bacteria placed in the rows DemSPBal[[i]] of the "especie".

Value

Returns a vector where the first component is a 1 and the following components have the values of the SPBal. The SPBal in the component $i+1$ has at its numerator the bacteria placed in the rows Num[[i]] of the especie. The SPBal of the component $i+1$ has at its denominator the bacteria placed in the rows Dem[[i]] of the especie.

References

Creus-Martí, I., Moya, A., Santonja, F. J. (2022). Bayesian hierarchical compositional models for analysing longitudinal abundance data from microbiome studies. *Complexity*, 2022.

Examples

```
v=c(0.1,0.1,0.2,0.3,0.3)
Num2<-list(3,c(3,5),1,c(3,5,4))
Dem2<-list(5,4,2,c(1,2))
MatrizPBmodelo=rbind(c(1,1,1,1),
                      c(-0.3,0.2,0.5,0.6),
                      c(-0.4,0.3,0.5,0.6),
                      c(0.5,0.3,0.2,0.7),
                      c(-0.2,0.9,0.2,0.1) )

FVectorPBmodeloPredi(Num2, Dem2, v, MatrizPBmodelo)
```

 Graphics

Plots the time series

Description

Plots the time series

Usage

```
Graphics(especie, names.especie, esperanza, Variance, Plot.Tipe, Detail)
```

Arguments

especie	Matrix that contains at row <i>i</i> the bacterial taxa of bacteria <i>i</i> at all time points.
names.especie	Vector with the names of the bacteria in the same order that are placed in the <i>especie</i> matrix.
esperanza	Matrix that contains at row <i>i</i> the expected value of the bacterial taxa <i>i</i> at all time points. The bacteria must be placed in the same order than in <i>especie</i>
Variance	Matrix that contains at row <i>i</i> the variance of the bacterial taxa <i>i</i> at all time points. The bacteria must be placed in the same order than in <i>especie</i>
Plot.Tipe	Character. If <i>Plot.Tipe</i> ==Data the function displays a graphic of the dataset, if <i>Plot.Tipe</i> ==DataExpected the function displays a graphic of the data and the expected values, if <i>Plot.Tipe</i> ==All the function displais a graphic with the data, the expected values and the variance.If <i>Plot.Tipe</i> ==Var the function returns the boxplot of the variance at each time point and the variance of each bacteria. If <i>Plot.Tipe</i> ==OnlyVar the function returns the boxplots of the variance at each time points.
Detail	Character. If <i>Detail</i> ==no the graphic obtained when <i>Plot.Tipe</i> ==DataExpected and <i>Plot.Tipe</i> ==All will have the same y axis for all the taxa. If <i>Detail</i> ==yes these functions will have different y axis.

Value

Returns the indicated plots.

Examples

```
names.especie=c("Bact1", "Bact2", "Bact3")
especie=cbind(c(0.5,0.3,0.2), c(0.6,0.3,0.1),c(0.4,0.1,0.5),c(0.4,0.1,0.5))
esperanza=especie[,c(1:3)]+0.1
Variance=matrix(c(runif(9,0.001,0.004)), 3,3)

Graphics(especie, names.especie, esperanza, Variance,"Data","no")
Graphics(especie, names.especie, esperanza, Variance,"DataExpected","no")
Graphics(especie, names.especie, esperanza, Variance,"All","no")
```

GraphicsPrediction *Plots the time series*

Description

This function takes into account the data used to estimate and the data used to predict.

Usage

```
GraphicsPrediction(
  especie.All,
  names.especie,
  ExpectedValue.All,
  VarianceValue.All,
  Pred,
  Plot.Tipe,
  Detail
)
```

Arguments

`especie.All` Matrix that contains at row *i* the bacterial taxa of bacteria *i* at all time points.

`names.especie` Vector with the names of the bacteria in the same order that are placed in the `especie` matrix.

`ExpectedValue.All`
 Matrix that contains at row *i* the expected value of the bacterial taxa *i* at all time points. The bacteria must be placed in the same order than in `especie`. This matrix must comply: $\text{dim}(\text{ExpectedValue.All})[2]=\text{dim}(\text{especie.All})[2]-1$

`VarianceValue.All`
 Matrix that contains at row *i* the variance of the bacterial taxa *i* at all time points. The bacteria must be placed in the same order than in `especie`. This matrix must comply: $\text{dim}(\text{VarianceValue.All})[2]=\text{dim}(\text{especie.All})[2]-1$

Pred	Number. Indicates the time point in which we start predicting.
Plot.Type	Character. If Plot.Type==Data the function displays a graphic of the dataset, if Plot.Type==DataExpected the function displays a graphic of the data and the expected values, if Plot.Type==All the function displays a graphic with the data, the expected values and the variance.If Plot.Type==Var the function returns the boxplot of the variance at each time point and the variance of each bacteria. If Plot.Type==OnlyVar the function returns the boxplots of the variance at each time points.
Detail	Character. If Detail==no the graphic obtained when Plot.Type==DataExpected and Plot.Type==All will have the same y axis for all the taxa. If Detail==yes these functions will have different y axis.

Value

Returns the indicated plots with a vertical line when the time point is equal to Pred-1, in Pred the prediction has started.

Examples

```
names.especie=c("Bact1", "Bact2", "Bact3")
especie.All=cbind(c(0.5,0.3,0.2),
                 c(0.6,0.3,0.1),
                 c(0.4,0.1,0.5),
                 c(0.4,0.1,0.5),
                 c(0.4,0.1,0.5),
                 c(0.4,0.1,0.5))
ExpectedValue.All=especie.All[,-1]+0.1
VarianceValue.All=matrix(c(runif(15,0.001,0.004)), 3,5)
Pred=4
```

```
GraphicsPrediction(especie.All,
                  names.especie,
                  ExpectedValue.All,
                  VarianceValue.All ,
                  Pred,
                  "Data",
                  "no")
```

```
GraphicsPrediction(especie.All,
                  names.especie,
                  ExpectedValue.All,
                  VarianceValue.All ,
                  Pred,
                  "DataExpected",
                  "no")
```

```
GraphicsPrediction(especie.All,
                  names.especie,
                  ExpectedValue.All,
                  VarianceValue.All ,
```

```

        Pred,
        "All",
        "no")

GraphicsPrediction(especie.All,
                  names.especie,
                  ExpectedValue.All,
                  VarianceValue.All ,
                  Pred,
                  "Var",
                  "no")

GraphicsPrediction(especie.All,
                  names.especie,
                  ExpectedValue.All,
                  VarianceValue.All ,
                  Pred,
                  "OnlyVar",
                  "no")

```

GraphicsPredictionBPBM

Plots the time series

Description

This function takes into account the data used to estimate and the data used to predict. We use this function when we want to observe the results obtained with the BPBM model.

Usage

```

GraphicsPredictionBPBM(
  especie.All,
  names.especie,
  ExpectedValue.All,
  VarianceValue.All,
  Pred,
  Plot.Tipe,
  Varmas,
  Varmenos,
  Detail
)

```

Arguments

`especie.All` Matrix that contains at row *i* the bacterial taxa of bacteria *i* at all time points.

<code>names.especie</code>	Vector with the names of the bacteria in the same order that are placed in the <code>especie</code> matrix.
<code>ExpectedValue.All</code>	Matrix that contains at row i the expected value of the bacterial taxa i at all time points. The bacteria must be placed in the same order than in <code>especie</code> . This matrix must comply: $\dim(\text{ExpectedValue.All})[2]=\dim(\text{especie.All})[2]-1$
<code>VarianceValue.All</code>	Matrix that contains at row i the variance of the bacterial taxa i at all time points. The bacteria must be placed in the same order than in <code>especie</code> . This matrix must comply: $\dim(\text{VarianceValue.All})[2]=\dim(\text{especie.All})[2]-1$
<code>Pred</code>	Number. Indicates the time point in which we start predicting.
<code>Plot.Type</code>	Character. If <code>Plot.Type==Data</code> the function displays a graphic of the dataset, if <code>Plot.Type==DataExpected</code> the function displays a graphic of the data and the expected values, if <code>Plot.Type==All</code> the function displays a graphic with the data, the expected values and the variance (the <code>varmas</code> and <code>varmenos</code> parameters are introduced and are taken into account to plot the variance of the predicted part). If <code>Plot.Type==Var</code> the function returns the boxplot of the variance at each time point and the variance of each bacteria. If <code>Plot.Type==OnlyVar</code> the function returns the boxplots of the variance at each time points.
<code>Varmas</code>	Matrix. Output of "PredictionBPBM" adding " <code>\$ExpVarmas</code> ". Matrix that contains at row i the expected value plus two times the $\sqrt{\text{variance}}$ of the bacteria i at all time points $t=Tt, \dots, K$, the rest of the time points has 0 values. The bacteria are placed at the same order than in <code>especies</code> .
<code>Varmenos</code>	Matrix. Output of "PredictionBPBM" adding " <code>\$ExpVarmenos</code> ". Matrix that contains at row i the expected value minus two times the $\sqrt{\text{variance}}$ of the bacteria i at all time points $t=Tt, \dots, K$, the rest of the time points has 0 values. The bacteria are placed at the same order than in <code>especies</code> .
<code>Detail</code>	Character. If <code>Detail==no</code> the graphic obtained when <code>Plot.Type==DataExpected</code> and <code>Plot.Type==All</code> will have the same y axis for all the taxa. If <code>Detail==yes</code> these functions will have different y axis.

Value

Returns the indicated plots with a vertical line when the time point is equal to $Tt=\text{Pred}-1$, in $\text{Pred}=Tt+1$ the prediction has started.

References

Creus-Martí, I., Moya, A., Santonja, F. J. (2022). Bayesian hierarchical compositional models for analysing longitudinal abundance data from microbiome studies. *Complexity*, 2022.

Examples

```
names.especie=c("Bact1", "Bact2", "Bact3")
especie.All=cbind(c(0.5,0.3,0.2),
                 c(0.6,0.3,0.1),
                 c(0.4,0.1,0.5),
```

```

      c(0.4,0.1,0.5),
      c(0.4,0.1,0.5),
      c(0.4,0.1,0.5))
ExpectedValue.All=especie.All[,-1]+0.1
VarianceValue.All=matrix(c(runif(15,0.001,0.004)), 3,5)
Pred=4
Varmas=cbind(matrix(0,3,2),matrix(c(runif(9,0.001,0.004)) ,3 ,3 ))
Varmenos=cbind(matrix(0,3,2),matrix(c(runif(9,0.001,0.004)) ,3 ,3 ))

GraphicsPredictionBPBM(especie.All,
      names.especie,
      ExpectedValue.All,
      VarianceValue.All ,
      Pred ,
      "Data",
      Varmas,
      Varmenos,
      "no")

GraphicsPredictionBPBM(especie.All,
      names.especie,
      ExpectedValue.All,
      VarianceValue.All ,
      Pred ,
      "DataExpected",
      Varmas,
      Varmenos,
      "no")

GraphicsPredictionBPBM(especie.All,
      names.especie,
      ExpectedValue.All,
      VarianceValue.All,
      Pred ,
      "All",
      Varmas,
      Varmenos,
      "no")

GraphicsPredictionBPBM(especie.All,
      names.especie,
      ExpectedValue.All,
      VarianceValue.All ,
      Pred ,
      "Var",
      Varmas,
      Varmenos,
      "no")

GraphicsPredictionBPBM(especie.All,
      names.especie,
      ExpectedValue.All,
      VarianceValue.All ,

```

```
Pred ,
"OnlyVar",
Varmas,
Varmenos,
"no")
```

GraphicsSPBal

Obtaining the graphic of the SPBal at all time points

Description

The SPBal (of BPBM model) are ordered from highest to lowest variance percentage. The zero is highlight because the closer the value of the balance is to zero, the more similar (in terms of relative abundance) the numerator and denominator groups will be. The farther away from zero, the more different.

Usage

```
GraphicsSPBal(MatrizPBmodelo)
```

Arguments

MatrizPBmodelo Matrix. Output of "ObtainigValueSPBal" function. MatrixSPBal is the matrix that contains the covariates of the model. The first line es equal to 1 for all columns. The other rows contain the value of one SPBal at all time points. The selected principal balance of the row $i+1$ has at its numerator the bacteria placed in the rows NumSPBal[[i]] of the "especie". The selected principal balance of the row $i+1$ has at its denominator the bacteria placed in the rows DemSPBal[[i]] of the "especie".

Value

Returns a graphic.

References

Creus-Martí, I., Moya, A., Santonja, F. J. (2022). Bayesian hierarchical compositional models for analysing longitudinal abundance data from microbiome studies. Complexity, 2022.

Examples

```
MatrizPBmodelo=rbind(c(1,1,1,1,1,1),c(-0.3,0.4,0.3,-0.7,-0.4,-0.6),c(0.3,0.5,-0.3,0.1,0.4,0.1))
GraphicsSPBal(MatrizPBmodelo)
```

LogVeroFuncBUENA *Writting the loglikelihood of the dirichlet*

Description

This function calculates the loglikelihood of the dirichlet for the BPBM model.

Usage

```
LogVeroFuncBUENA(param, MatrizPBmodelo, E, Tt, especiemodi)
```

Arguments

param	Vector. Column "mean" of the output of "StudyingParam" function.
MatrizPBmodelo	Matrix with the covariates of the model. In an example with two SPBal and three time points, the covariates are written in the following order:
	$\begin{matrix} & 1 & & 1 & & 1 \\ & SPBal_{1,t-1} & & SPBal_{1,t-2} & & SPBal_{1,t-3} \\ & SPBal_{2,t-1} & & SPBal_{2,t-2} & & SPBal_{2,t-3} \end{matrix}$
E	Number f bacteria in the dataset.
Tt	Number of time points available
especiemodi	Matrix that contains at row i the bacterial taxa of bacteria i at time points t=2,...,Tt.

Value

Returns a number with the value of the dirichlet loglikelihood.

References

Creus-Martí, I., Moya, A., Santonja, F. J. (2022). Bayesian hierarchical compositional models for analysing longitudinal abundance data from microbiome studies. *Complexity*, 2022.

Examples

```
set.seed(314)
especie=t(gtools::rdirichlet(n=2, c(1,2,3)))
E=3
Tt=2
MatrizPBmodelo=rbind(c(1,1),c(-0.3,0.4),c(0.3,0.5))
set.seed(314)
est=Estimating_BPBM(especie,
                    Tt,
                    E,
                    MatrizPBmodelo,
                    nn.chain=3,
```

```

nn.burnin=1000,
nn.sample=5000,
nn.thin=10)

param=est$SamplesAllChains

especiemodi=especie[,-1]

LogVeroFuncBUENA(param,MatrizPBmodelo,E,Tt,especiemodi)

```

MaxBacteria	<i>Putting the reference bacteria at the last row</i>
-------------	---

Description

This function calculates the mean abundance of each bacteria. Then, it creates a matrix where each row contains the abundance of one bacteria at all time points but the bacteria with maximum (or minimum or a bacteria indicated by the user) mean abundance is placed at the last row

Usage

```
MaxBacteria(nombresOriginal, especieOriginal, E, Tt, which.esp)
```

Arguments

nombresOriginal	Vector with the bacterial names at the same order than in DaTa. it must be fulfilled that $\text{lenght}(\text{nombresOriginal}) == \text{dim}(\text{DaTa})[2]-1$
especieOriginal	Matrix that contains at row i the bacterial taxa of bacteria i at all time points
E	Number of bacteria available
Tt	Number of bacteria available
which.esp	If $\text{which} == \text{"Max"}$ this function puts in the last position of the matrix the bacteria with maximum mean abundance. If $\text{which} == \text{"Min"}$ this function puts in the last position of the matrix the bacteria with minimum mean abundance. If which is equal to a number this function puts in the last position of the matrix the bacteria that is in the "which" row of the especieOriginal matrix.

Value

Returns a list with

- especie - Matrix that contains at row i the bacterial taxa of bacteria i at all time points but the bacteria with maximum (or minimum) mean abundance (or the bacteria indicated by the user) is placed at the last row.

- `especiemodi` - Matrix that contains at row i the bacterial taxa of bacteria i at time points $t=2, \dots, Tt$ but the bacteria with maximum (or minimum) mean abundance (or the bacteria indicated by the user) is placed at the last row.
- `nombres` - Vector with the bacteria's names placed in the order in which appear in the rows of the matrices `especie` and `especiemodi`
- `EE` - Row in which the bacterial with maximum (or minimum) mean abundance was (or the value of "which" if which is numerical).
- `EspecieMaxima` - Row in which the bacterial with maximum (or minimum) mean abundance (or the bacteria indicated by the user) is in `especie`.) #'

Examples

```
names1=c("Bact1", "Bact2", "Bact3")
set.seed(314)
esp1=t(gtools::rdirichlet(n=4, c(1,3,1)))
e1=3
t1=4
```

```
MaxBacteria(names1,esp1,e1,t1,"Max")
```

```
names3=c("Bact1", "Bact2", "Bact3", "Bact4", "Bact5")
set.seed(314)
esp3=t(gtools::rdirichlet(n=6, c(6,6,1,6,6)))
e3=5
t3=6
MaxBacteria(names3,esp3,e3,t3,"Min")
```

MaxBacteriaPred

Putting the reference bacteria at the last row

Description

This function calculates the mean abundance of each bacteria taking into account the time points used to estimate the model ($t=1,2,\dots,Tt$). Then, it creates a matrix where each row contains the abundance of one bacteria at all time points but the bacteria with maximum (or minimum) mean abundance (or the bacterial indicated by the user) is placed at the last row

Usage

```
MaxBacteriaPred(
  nombresOriginal,
  especieOriginal,
  E,
  Tt,
  Pred,
```

```

    K,
    especieOriginal.All,
    which.esp
)

```

Arguments

`nombresOriginal` Vector with the bacterial names at the same order than in `DaTa`. it must be fulfilled that `length(nombresOriginal)==dim(DaTa)[2]-1`

`especieOriginal` Matrix that contains at row *i* the bacterial taxa of bacteria *i* at $t=1,2,\dots,Tt$, with $Tt=Pred-1$.

`E` Number of bacteria available

`Tt` Number of time points used to estimate the model ($Tt=Pred-1$)

`Pred` Number. The data at $t=1,\dots,Pred-1$ will be used to estimate the model. The rest of the time points will be used to study the capacity of the model to predict. If $Pred==0$ all the dataset will be used to estimate the model.

`K` Number of time points at the data

`especieOriginal.All` Matrix that contains at row *i* the bacterial taxa of bacteria *i* at all time points.

`which.esp` If `which=="Max"` this function puts in the last position of the matrix the bacteria with maximum mean abundance. If `which=="Min"` this function puts in the last position of the matrix the bacteria with minimum mean abundance. If `which` is equal to a number this function puts in the last position of the matrix the bacteria that is in the "which" row of the `especieOriginal` matrix.

Value

Returns a list with

- `especie` - Matrix that contains at row *i* the bacterial taxa of bacteria *i* at time points $t=1,2,\dots,Tt$ but the bacteria with with maximum (or minimum) mean abundance (or the bacteria indicated by the user) is placed at the last row.
- `especiemodi` - Matrix that contains at row *i* the bacterial taxa of bacteria *i* at time points $t=2,\dots,Tt$ but the bacteria with with maximum (or minimum) mean abundance (or the bacteria indicated by the user) is placed at the last row.
- `nombres` - Vector with the bacteria's names placed in the order in which appear in the rows of the matrices `especie` and `especiemodi`
- `EE` - Row in which the bacterial with maximum (or minimum) mean abundance was (or the value of "which" if which is numerical).
- `EspecieMaxima` - Row in which the bacterial with with maximum (or minimum) mean abundance (or the bacteria indicated by the user) is in `especie`.) #' #'
- `especie.all` - Matrix that contains at row *i* the bacterial taxa of bacteria *i* at all time points ($t=1,2,\dots,K$) but the bacteria with with maximum (or minimum) mean abundance (or the bacteria indicated by the user) is placed at the last row.

- `especiemodi.all` - Matrix that contains at row i the bacterial taxa of bacteria i at all time points ($t=2,\dots,K$) but the bacteria with with maximum (or minimum) mean abundance (or the bacteria indicated by the user) is placed at the last row.

Examples

```
names2=c("Bact1","Bact2","Bact3","Bact4","Bact5")
set.seed(314)
esp2=t(gtools::rdirichlet(n=6, c(1,1,5,1,1)))
e2=5

MaxBacteriaPred(names2,esp2[, -c(4,5,6)],e2,3,Pred=4, 6,esp2, "Max")
```

ObtainigValuePB

Obtaining the principal balances values

Description

Calculates the value of the principal balances (Martín-Fernández et al, 2018) at all time points.

Usage

```
ObtainigValuePB(Num, Dem, especie, Tt)
```

Arguments

Num	List. The component i of the list has the number of the row of the matrix <code>especie</code> where the bacteria in the numerator of the principal balance i are placed.
Dem	List. The component i of the list has the number of the row of the matrix <code>especie</code> where the bacteria in the denominator of the principal balance i are placed.
<code>especie</code>	Matrix that contains at row i the bacterial taxa of bacteria i at all time points.
Tt	Number of time points available

Value

Returns a matrix where the row i has the value of the principal balance at all time points. The principal balance of the row i has at its numerator the bacteria placed in the rows `Num[[i]]` of the `especie`. The principal balance of the row i has at its denominator the bacteria placed in the rows `Dem[[i]]` of the `especie`.

References

- Creus-Martí, I., Moya, A., Santonja, F. J. (2022). Bayesian hierarchical compositional models for analysing longitudinal abundance data from microbiome studies. *Complexity*, 2022.
- Martín-Fernández, J. A., Pawlowsky-Glahn, V., Egozcue, J. J., & Tolosona-Delgado, R. (2018). Advances in principal balances for compositional data. *Mathematical Geosciences*, 50, 273-298.

Examples

```
set.seed(314)
esp2=t(gtools::rdirichlet(n=6, c(1,1,5,1,1)))

Num2<-list(3,c(3,5),1,c(3,5,4))
Dem2<-list(5,4,2,c(1,2))

ObtainigValuePB(Num2, Dem2, esp2, 6)
```

ObtainigValueSPBal *Obtaining the selected principal balances values*

Description

Calculates the value of the selected principal balances (SPBal) of the BPBM model at all time points.

Usage

```
ObtainigValueSPBal(Num, Dem, especie, Tt)
```

Arguments

Num	List. The component i of the list has the number of the row of the matrix <i>especie</i> where the bacteria in the numerator of the principal balance i are placed.
Dem	List. The component i of the list has the number of the row of the matrix <i>especie</i> where the bacteria in the denominator of the principal balance i are placed.
<i>especie</i>	Matrix that contains at row i the bacterial taxa of bacteria i at all time points.
Tt	Number of time points available

Value

Returns a list with:

- NumSPBal: List. The component i of the list has the number of the row of the matrix `especie` where the bacteria in the numerator of the selected principal balance i are placed.
- DemSPBal: List. The component i of the list has the number of the row of the matrix `especie` where the bacteria in the denominator of the selected principal balance i are placed.
- MatrixSPBal: MatrixSPBal is the matrix that contains the covariates of the model. The first line es equal to 1 for all columns. The other rows contain the value of one SPBal at all time points. The selected principal balance of the row $i+1$ has at its numerator the bacteria placed in the rows NumSPBal[[i]] of the "especie". The selected principal balance of the row $i+1$ has at its denominator the bacteria placed in the rows DemSPBal[[i]] of the "especie".
- PercenVarianceSPBal: Vector. The component of the vector i contains the percentage of variance of the SPBal with numerator NumSPBal[[i]] and denominator DemSPBal[[i]].

References

Creus-Martí, I., Moya, A., Santonja, F. J. (2022). Bayesian hierarchical compositional models for analysing longitudinal abundance data from microbiome studies. *Complexity*, 2022.

Examples

```
set.seed(314)
esp2=t(gtools::rdirichlet(n=6, c(1,1,5,1,1)))

Num2<-list(3,c(3,5),1,c(3,5,4))
Dem2<-list(5,4,2,c(1,2))

ObtainigValueSPBal(Num2, Dem2, esp2, 6)
```

ObtainingDIC

Writting the loglikelihood of the dirichlet

Description

This function calculates the loglikelihood of the dirichlet for the BPBM model. Then, it calculates the loglikelihood with the parameters of each iteration of the MCMC chains and introduces the values in a vector called vectorD. $DIC=(1/2)*var(vectorD)+mean(VectorD)$

Usage

```
ObtainingDIC(cadenas, MatrizPBmodelo, E, Tt, especiemodi)
```

Arguments

cadena	Matrix with the iterations (in rows) of all the Markov Chains obtained in the estimation. It is the output of "StudyingParam" adding "\$AllChainsJoined".
MatrizPBmodelo	Matrix with the covariates of the model. In an example with two SPBal and three time points, the covariates are written in the following order:
	$\begin{matrix} & 1 & & 1 & & 1 \\ SPBal_{1,t-1} & & SPBal_{1,t-2} & & SPBal_{1,t-3} \\ SPBal_{2,t-1} & & SPBal_{2,t-2} & & SPBal_{2,t-3} \end{matrix}$
E	Number of bacteria in the dataset.
Tt	Number of time points available
especiemodi	Matrix that contains at row i the bacterial taxa of bacteria i at time points t=2,...,Tt.

Value

Returns a data.frame with the DIC value (using the rule, $pD = \text{var}/2$).

References

Creus-Martí, I., Moya, A., Santonja, F. J. (2022). Bayesian hierarchical compositional models for analysing longitudinal abundance data from microbiome studies. *Complexity*, 2022.

Examples

```

set.seed(314)
especie=t(gtools::rdirichlet(n=2, c(1,2,3)))
E=3
Tt=2
MatrizPBmodelo=rbind(c(1,1),c(-0.3,0.4),c(0.3,0.5))
set.seed(314)
est=Estimating_BPBM(especie,
                    Tt,
                    E,
                    MatrizPBmodelo,
                    nn.chain=3,
                    nn.burnin=1000,
                    nn.sample=5000,
                    nn.thin=10)
SumFinal=StudyingParam(est$R2jagsOutput$BUGSoutput$summary, est$SamplesAllChains)
cadena=SumFinal$AllChainsJoined
especiemodi=especie[,-1]

ObtainingDIC(cadena,MatrizPBmodelo,E,Tt,especiemodi)

```

PBalance *Calculating balances*

Description

This function calculates the balance that has at the numerator the bacteria placed at Num and has at the denominator the bacteria placed at Dem

Usage

```
PBalance(A, Num, Dem, especie)
```

Arguments

A	Number. The balance will be calculated for $t=1,2,\dots,A$ time points.
Num	vector that contains the position in the matrix especies of the families that we position at the numerator of the balance.
Dem	vector that contains the position in the matrix especies of the families that we position at the denominator of the balance
especie	Matrix that contains at row i the bacterial taxa of bacteria i at all time points.

Value

Returns a vector with the value of the balance in each time point.

Examples

```
especie1=cbind(c(0.5,0.3,0.1,0.1), c(0.1,0.3,0.6,0.1))
Num=c(1,2)
Dem=c(3,4)
A=2
PBalance(A,Num,Dem,especie1)
```

PBalancePredi *Calculating balances for a composition*

Description

This function calculates the balance that has at the numerator de bacteria placed at Num and has at the denominator the bacteria placed at Dem

Usage

```
PBalancePredi(Num, Dem, DatosEsperanzas)
```

Arguments

Num	vector that contains the position in the matrix especies of the families that we position at the numerator of the balance.
Dem	vector that contains the position in the matrix especies of the families that we position at the denominator of the balance
DatosEsperanzas	Vector with a coda composition. The bacteria are in the same orden than the matrix especie

Value

Returns the value of the balance

Examples

```
Num=c(1,2)
Dem=c(3,4)
DatosEsperanzas=c(0.1,0.3,0.4,0.2)

PBalancePredi(Num, Dem, DatosEsperanzas)
```

PBmodel

Obtaining the regression value of the BPBM

Description

This function calculates the value of the BPBM regression, defined by:

$$\mu_{it} = a_{i0} + a_{i1} \cdot \text{SPBal}_{1,t-1} + \dots + a_{iM} \cdot \text{SPBal}_{M,t-1}$$

Usage

```
PBmodel(A, MatrizPBmodelo, E, Tt)
```

Arguments

A Matrix that contains all the parameters of the model. The parameters are written in the matrix in the following order (in an example with three bacteria):

```

a10 a11 a12 ... a1M
a20 a21 a22 ... a2M
a30 a31 a32 ... a3M
```

MatrizPBmodelo Matrix. Output of "ObtainingValueSPBal" called "MatrixSPBal".

E Number of bacteria in the dataset.

Tt Number of time points.

Value

Returns a matrix. The row i contains the regression values of the bacteria i at all time points.

References

Creus-Martí, I., Moya, A., Santonja, F. J. (2022). Bayesian hierarchical compositional models for analysing longitudinal abundance data from microbiome studies. *Complexity*, 2022.

Examples

```
A=rbind(c(1,2,3),c(4,5,6),c(7,8,9))
MatrizPBmodelo=cbind(c(1,2,3),c(4,5,6),c(7,8,9))
E=3
Tt=3

PBmodel(A,MatrizPBmodelo, E,Tt)
```

PCAbiplot

PCA of the estimated parameters

Description

This function applies a PCA to the estimate parameters (using function "prcomp" with center = TRUE and scale. = TRUE). Then uses the ggbiplot function to plot the biplot.

Usage

```
PCAbiplot(paramEstimadosFinal, names, E)
```

Arguments

paramEstimadosFinal	The estimate parameters, in the following order: $a_{11}, a_{12}, a_{13}, a_{21}, a_{22}, a_{23}, \dots, a_{(D-1)1}, a_{(D-1)2}, a_{(D-1)3}, \tau$. Where D is the number of bacterial species present in the matrix especie.
names	Vector with the name of the bacteria. The component i has the name of the bacteria i , with $i=1, \dots, D$. The bacteria in the last position of the vector is the bacteria used as reference in the alr transformation.
E	Number of bacteria available.

Value

Returns a list with the PCA biplot, the variance explained of each Principal Component and an object of class "prcomp" with the PCA. In the biplot, "a" denotes the intercept, "b" denotes the parameter that give information about the importance of the bacteria in defining herself in the next time point and "c" denotes denotes the parameter that give information about the importance of the rest of the community in defining the bacteria in the next time point.

Examples

```
set.seed(123)
especie=t(gtools::rdirichlet(10,c(1,3,1,2,4)))
names=c("Bact1","Bact2","Bact3","Bact4","Bact5")
tau1=0.4
parms1= cbind(c(0.1,0.2,0.4,0.6),c(-0.2,0.1,0.1,0.3),c(0.3,0.2,0.3,0.5))
paramEstimadosFinal=c(as.vector( t(parms1)),tau1)

PCAbiplot(paramEstimadosFinal,names,5)
```

Percen_Variance	<i>Percentage of variance</i>
-----------------	-------------------------------

Description

This function calculates the variance of each row of the matrix PB. Returns the percentage of variance of each row of the matrix PB.

Usage

```
Percen_Variance(PB)
```

Arguments

PB Matrix.

Value

Returns a vector with percentage of variance of each row of the matrix PB.

Examples

```
matt=matrix(c(1:4),2,2)
```

```
Percen_Variance(matt)
```

PlotDendogram *Plotting a dendogram*

Description

Plots the dendogram obtained using the Ward's method for obtaining the principal balances. The process follow in this function is explained in Section 3.1 of (Creus-Martí et al, 2022)

Usage

```
PlotDendogram(especie, names)
```

Arguments

especie	Matrix that contains at row i the bacterial taxa of bacteria i at all time points.
names	Vector with the names of the bacteria in the same order that are written in especie.

Value

Returns a list with: the dendogram.

- Num: List. The component i of the list has the number of the row of the matrix especie where the bacteria in the numerator of the principal balance i are placed.
- Dem: List. The component i of the list has the number of the row of the matrix especie where the bacteria in the denominator of the principal balance i are placed.
- dendogram: Plots the dendogram.

References

Creus-Martí, I., Moya, A., Santonja, F. J. (2022). Bayesian hierarchical compositional models for analysing longitudinal abundance data from microbiome studies. *Complexity*, 2022.

Examples

```
names2=c("Bact1", "Bact2", "Bact3", "Bact4", "Bact5")
set.seed(314)
esp2=t(gtools::rdirichlet(n=6, c(1,1,5,1,1)))
```

```
PlotDendogram(esp2, names2)
```


Description

This function calculates the expected value and variance of the bacteria at time point T_t . Then, this function calculates the expected value and variance of the bacteria at time point $t=(T_t+1), \dots, K$. It calculates the expected value at each time point for each markov chain iteration. The expected value for each time point is the mean of the expected values of all iterations. Analogous with the variance, the dirichlet parameters and the expected value plus (and minus) two times the sqrt of the variance.

Usage

```
PredictionBPBM(
  NumSPBal,
  DemSPBal,
  MCMC.CHAINS,
  alpha,
  K,
  esperanza,
  Var,
  E,
  Tt,
  MatrizPBmodelo
)
```

Arguments

NumSPBal	List. The component i of the list has the number of the row of the matrix especie where the bacteria in the numerator of the principal balance i are placed.
DemSPBal	List. The component i of the list has the number of the row of the matrix especie where the bacteria in the denominator of the principal balance i are placed.
MCMC.CHAINS	Matrix with the iterations of all the chains for all the parameters. Each column has all the iteration of one parameter. If the zero is in the center of the credible interval of one parameter all its iteration in the Markov Chain have the value 0. It is output of the "StudyingParam" function adding "\$AllChainsJoined".
alpha	Matrix that contains at the row i the Dirichlet parameter of the bacteria i at $t=1,2,3,\dots,T_t$.
K	Number. The function will calculate the value of the expected value and the variance at T_t and predict for the time points $t=T_t+1,\dots,K$. To predict all the time points available at the data we $K=\dim(\text{especie.All})-1$
esperanza	Matrix that contains at row i the expected value of the bacterial taxa of bacteria i at $t=1,2,3,\dots,T_t-1$.

Var	Matrix that contains at row i the variance of the bacterial taxa of bacteria i at $t=1,2,3,\dots,Tt-1$.
E	Number of bacteria available
Tt	Number of bacteria available
MatrizPBmodelo	is the matrix that contains the covariates of the model. The first line es equal to 1 for all columns. The other rows contain the value of one SPBal at all time points. The selected principal balance of the row $i+1$ has at its numerator the bacteria placed in the rows NumSPBal[[i]] of the "especie". The selected principal balance of the row $i+1$ has at its denominator the bacteria placed in the rows DemSPBal[[i]] of the "especie".

Value

Returns a list with:

- **ExpectedValue.All:** Matrix. Matrix that contains at row i the expected value of the bacteria i at all time points $t=1,2,\dots,K$. The bacterias are placed at the same order than in especies.
- **VarianceValue.All:** Matrix. Matrix that contains at row i the variance of the bacteria i at all time points $t=1,2,\dots,K$. The bacterias are placed at the same order than in especies.
- **DirichlerParam.All:** Matrix. Matrix that contains at row i the dirichlet parameter of the bacteria i at all time points $t=1,2,\dots,K$. The bacterias are placed at the same order than in especies.
- **ExpVarmas:** Matrix. Matrix that contains at row i the expected value plus two times the $\sqrt{\text{variance}}$ of the bacteria i at all time points $t=Tt,\dots,K$, the rest of the time points has 0 values. The bacterias are placed at the same order than in especies.
- **ExpVarmenos:** Matrix. Matrix that contains at row i the expected value plus two times the $\sqrt{\text{variance}}$ of the bacteria i at all time points $t=Tt,\dots,K$, the rest of the time points has 0 values. The bacterias are placed at the same order than in especies.

References

Creus-Martí, I., Moya, A., Santonja, F. J. (2022). Bayesian hierarchical compositional models for analysing longitudinal abundance data from microbiome studies. *Complexity*, 2022.

Examples

```

NumSPBal=list(1,c(1,2))
DemSPBal=list(2,3)
MCMC.CHAINS=cbind(c(0.1,0.11),
                  c(0.2,0.21),
                  c(0.3,0.31),
                  c(-0.1,-0.11),
                  c(0.15,0.105),
                  c(0.44,0.41),
                  c(0.3,0.31),
                  c(0.201,0.221),
                  c(0.13,0.113) )
alpha=cbind(c(0.1,0.2,0.1),c(0.1,0.5,0.3))
K=3

```

```

esperanza=cbind(c(0.2,0.2,0.6))
Var=cbind(c(0.1,0.01,0.11))
E=3
Tt=2
MatrizPBmodelo=cbind(c(1,0.3,0.2))

PredictionBPBM(NumSPBal, DemSPBal, MCMC.CHAINS, alpha, K, esperanza, Var, E, Tt, MatrizPBmodelo )

```

PredictionEstParmFunc *Predicting using dirichl-gLV*

Description

This function calculates the expected value and variance of the bacteria at time point Tt. Then, this function calculates the expected value and variance of the bacteria at time point t=(Tt+1),...,K

Usage

```

PredictionEstParmFunc(
  paramEstimadosFinal,
  EspecieMaxima,
  alpha,
  K,
  esperanza,
  Var,
  E,
  Tt
)

```

Arguments

paramEstimadosFinal

The estimate parameters. Vector equal to $c(\tau, as.vector(pam))$ where:

- pam Matrix. Each row has the parameters of each bacteria. Following our example, pam has the parameters placed as follows:

```

r1  a11  a12
r2  a21  a22

```

- tau Number. Value of the tau parameter in the model

EspecieMaxima Row in which the bacteria chosen as reference is in especie. This bacteria is used as reference in the alr transformation that the model does.

alpha Matrix that contains at the row i the dirichlet parameter of the bacteria i at $t=1,2,3,\dots,Tt$.

K	Number. The function will calculate the value of the expected value and the variance at Tt and predict for the time points t=Tt+1,...,K. To predict all the time points available at the data we K=dim(especie.All)-1
esperanza	Matrix that contains at row i the expected value of the bacterial taxa of bacteria i at t=1,2,3,...,Tt-1.
Var	Matrix that contains at row i the variance of the bacterial taxa of bacteria i at t=1,2,3,...,Tt-1.
E	Number of bacteria available
Tt	Number of time points available

Details

The regression of this model, in an example with three bacteria, is defined by

$$r_1 \cdot \log(x_1(t)/x_3(t)) + \log(x_1(t)/x_3(t)) \cdot [a_{11} \cdot \log(x_1(t)/x_3(t))(t) + a_{12} \cdot \log(x_2(t)/x_3(t))] \\ r_2 \cdot \log(x_2(t)/x_3(t)) + \log(x_2(t)/x_3(t)) \cdot [a_{21} \cdot \log(x_1(t)/x_3(t))(t) + a_{22} \cdot \log(x_2(t)/x_3(t))]$$

Value

Returns a list with:

- ExpectedValue.All: Matrix. Matrix that contains at row i the expected value of the bacteria i at all time points t=2,...,K. The bacteria are placed at the same order than in especies.
- VarianceValue.All: Matrix. Matrix that contains at row i the variance of the bacteria i at all time points t=2,...,K. The bacteria are placed at the same order than in especies.
- DirichlerParam.All: Matrix. Matrix that contains at row i the dirichlet parameter of the bacteria i at all time points t=2,...,K. The bacteria are placed at the same order than in especies.

References

Creus-Martí, I. and Moya, A. and Santonja, F. J. (2018). A Statistical Model with a Lotka-Volterra Structure for Microbiota Data. Lucas Jodar, Juan Carlos Cortes and Luis Acedo, Modelling or engineering and human behavior 2018, Instituto Universitario de Matematica Multidisciplinar. ISBN: 978-84-09-07541-6

Examples

```
pam.ini=rbind(c(0.1,0.2,0.3),c(0.4,0.5,0.6))
paramEstimadosFinal=c(5, as.vector(pam.ini))
EspecieMaxima=3
alpha=cbind(c(2,2,3),c(1,1,3))
K=3
esperanza=cbind(c(0.2,0.3,0.5))
Var=cbind(c(0.2,0.3,0.5))
E=3
Tt=2
```

```
PredictionEstParmFunc(paramEstimadosFinal,EspecieMaxima, alpha,K,esperanza,Var,E,Tt )
```

 PredictionFBM

Predicting using FBM

Description

This function calculates the expected value and variance of the bacteria at time point Tt . Then, this function calculates the expected value and variance of the bacteria at time point $t=(Tt+1),\dots,K$

Usage

```
PredictionFBM(
  paramEstimadosFinal,
  EspecieMaxima,
  alpha,
  K,
  esperanza,
  Var,
  E,
  Tt
)
```

Arguments

paramEstimadosFinal	The estimate parameters, in the following order: $a_{11},a_{12},a_{13}, a_{21}, a_{22},a_{23}, \dots,a_{(D-1)1},a_{(D-1)2},a_{(D-1)3},\tau$. Where D is the number of bacterial species present in the matrix <i>especie</i> .
EspecieMaxima	Row in which the bacteria chosen as reference is in <i>especie</i> .This bacteria is used as reference in the alr transformation that the model does and it is placed at the denominator of the balance)
alpha	Matrix that contains at the row i the Dirichlet parameter of the bacteria i at $t=1,2,3,\dots,Tt$.
K	Number. The function will calculate the value of the expected value and the variance at Tt and predict for the time points $t=Tt+1,\dots,K$. To predict all the time points available at the data we $K=\dim(\text{especie.All})-1$
esperanza	Matrix that contains at row i the expected value of the bacterial taxa of bacteria i at $t=1,2,3,\dots,Tt-1$.
Var	Matrix that contains at row i the variance of the bacterial taxa of bacteria i at $t=1,2,3,\dots,Tt-1$.
E	Number of bacteria available
Tt	Number of bacteria available

Details

The regression of this model is defined by

$$\mu_{it} = a_{i1} + a_{i2} \cdot \text{alr}(x_{i,(t-1)}) + a_{i3} \cdot \text{Balance}(x_{i,(t-1)}) \text{ for } i = 1, \dots, D-1 \text{ where } D \text{ is the number of bacteria}$$

Value

Returns a list with:

- **ExpectedValue.All:** Matrix. Matrix that contains at row i the expected value of the bacteria i at all time points $t=1,2,\dots,K$. The bacteria are placed at the same order than in especies.
- **VarianceValue.All:** Matrix. Matrix that contains at row i the variance of the bacteria i at all time points $t=1,2,\dots,K$. The bacteria are placed at the same order than in especies.
- **DirichlerParam.All:** Matrix. Matrix that contains at row i the dirichlet parameter of the bacteria i at all time points $t=1,2,\dots,K$. The bacteria are placed at the same order than in especies.

References

Creus-Martí, I., Moya, A., Santonja, F. J. (2021). A Dirichlet autoregressive model for the analysis of microbiota time-series data. *Complexity*, 2021, 1-16.

Examples

```
Tt=2
E=3
tau=5
EspecieMaxima=3
K=3
parms11=c(0.1,0.2,0.3,0.4,0.5,0.6,tau)
alpha=cbind(c(1.726793,1.892901,1.380306),
            c(1,1,3))
Expected=cbind(c(alpha[1,1]/tau, alpha[2,1]/tau, alpha[3,1]/tau ),
              c(alpha[1,2]/tau,alpha[2,2]/tau,alpha[3,2]/tau))
Variance=cbind(c(0.03768101, 0.03920954, 0.03330857 ),
              c( 0.03683242,0.02784883, 0.0413761 ))
Expected.final=Expected[,-2]
Variance.final=Variance[,-2]

PredictionFBM(parms11,EspecieMaxima, alpha,K,Expected.final,Variance.final,E,Tt )
```

Description

Preparing the dataset to be introduced in the models' functions. In order to introduce the usage of the package there is a README file. You can find the link to the file using `base::system.file("extdata", "README.pdf", package = "CoDaLoMic")`. On windows you can open the file with `base::shell.exec(system.file("extdata", "README.pdf", package = "CoDaLoMic"))`.

Usage

```
PreparingTheData(DaTa, Pred)
```

Arguments

DaTa	data.frame. The first column contains the time point information (natural numbers 1,2,3...). The rest of the columns contain the relative abundance of each bacteria at the different time points. The values of each column must sum 1.
Pred	Number. The data at $t=1, \dots, \text{Pred}-1$ will be used to estimate the model. The rest of the time points will be used to study the capacity of the model to predict. If $\text{Pred}==0$ all the dataset will be used to estimate the model.

Value

If $\text{Pred}==0$ returns a list with

- Tt - The number of time points available.
- E - Number of bacteria available
- `especieOriginal` - Matrix that contains at row i the bacterial taxa of bacteria i at all time points.
- `especiemodiOriginal` - Matrix that contains at row i the bacterial taxa of bacteria i at time points $t=2, \dots, \text{Tt}$.

If $\text{Pred} \neq 0$ returns a list with

- Tt - The number of time points available used to estimate the model ($\text{Tt}=\text{Pred}-1$).
- E - Number of bacteria available
- `especieOriginal` - Matrix that contains at row i the bacterial taxa of bacteria i at the time points $t=1, 2, \dots, \text{Pred}-1$.
- `especiemodiOriginal` - Matrix that contains at row i the bacterial taxa of bacteria i at time points $t=2, \dots, \text{Pred}-1$.
- `especieOriginal.All` - Matrix that contains at row i the bacterial taxa of bacteria i at the time points.
- `especiemodiOriginal.All` - Matrix that contains at row i the bacterial taxa of bacteria i at time points.
- K - Number of time points available at the dataset.

Examples

```
df<-data.frame(cbind(c(1,2,3),
                    c(0.5,0.2,0.3),
                    c(0.2,0.1,0.6),
                    c(0.1,0.1,0.8),
                    c(0.3,0.3,0.4)))
PreparingTheData(df,Pred=0)

df2<-data.frame(cbind(c(1,2,3,4,5),
                    c(0.1,0.1,0.1,0.2,0.5),
                    c(0.2,0.2,0.2,0.2,0.2),
                    c(0.2,0.3,0.1,0.2,0.2)))
PreparingTheData(df2,Pred=4)
```

QualityControl

Analysing the quality of the estimation

Description

This function calculates the root-mean-square deviation (RMSD), the Nash Sutcliffe Coefficient, the residual sum of squares (RSS) and the mean absolute percentage error (MAPE) for the matrices introduces. This function also calculates the mean of the RMSD, the mean of the Nash Sutcliffe Coefficient and the mean of the RSS.

Usage

```
QualityControl(matrixData, matrixExpected, names.especie)
```

Arguments

<code>matrixData</code>	Matrix that contains at row <i>i</i> the bacterial taxa of bacteria <i>i</i> at the time points that we want take into account to calculate the quality control values.
<code>matrixExpected</code>	Matrix that contains at row <i>i</i> the expected value of the bacterial taxa <i>i</i> at the time points that we want take into account to calculate the quality control values. The bacteria must be placed in the same order than in <code>matrixData</code>
<code>names.especie</code>	Vector with the names of the bacteria in the same order that are placed in the <code>matrixData</code> matrix.

Value

Returns a data.frame.

Examples

```
names.especie=c("Bact1", "Bact2", "Bact3")
matrixExpected=matrix(c(1:9),3,3)
matrixData=matrixExpected+0.1

QualityControl(matrixData, matrixExpected,names.especie)
```

ridgeregression	<i>Ridge regression</i>
-----------------	-------------------------

Description

Ridge regression

Usage

```
ridgeregression(Tt, especie, E, EspecieMaxima, seed = NULL)
```

Arguments

Tt	Number of time points available
especie	Matrix that contains at row i the bacterial taxa of bacteria i at all time points. The bacteria placed in the last row of the matrix will be used as reference in the alr transformation and will be at the denominator of the balance.
E	Number of bacteria available.
EspecieMaxima	Row in which the bacteria used as reference is in especie. This is the bacteria that is going to be at the denominator of the balance and the denominator of the alr transformation. As a result, in this function, EspecieMaxima must be equal to E
seed	Number. Set a seed. Default seed=NULL.

Value

Returns the result of the ridge regression, object of class "ridgelm".

Examples

```
set.seed(123)
especie=t(gtools::rdirichlet(10,c(1,3,1,2,4)))
Tt=10
E=5
EspecieMaxima=5
```

```
ridgeregression(Tt,especie, E, EspecieMaxima, 558562316)
```

```
rxnrate
```

Solving the right side of the gLV equations

Description

This function calculates the right side of the gLV equation.

Usage

```
rxnrate(State, parms)
```

Arguments

State	Vector with a CoDa composition
parms	Matrix. Each row has the parameters of each differential equation. following our example, parms has the parameters placed as follows:

r1	a11	a12	a13
r2	a21	a22	a23
r3	a31	a32	a33

Details

For instance, if we want to solve the following gLV equations:

$$\frac{dx_1(t)}{dt} = r_1 \cdot x_1(t) + x_1(t) \cdot [a_{11} \cdot x_1(t) + a_{12} \cdot x_2(t) + a_{13} \cdot x_3(t)]$$

$$\frac{dx_2(t)}{dt} = r_2 \cdot x_2(t) + x_2(t) \cdot [a_{21} \cdot x_1(t) + a_{22} \cdot x_2(t) + a_{23} \cdot x_3(t)]$$

$$\frac{dx_3(t)}{dt} = r_3 \cdot x_3(t) + x_3(t) \cdot [a_{31} \cdot x_1(t) + a_{32} \cdot x_2(t) + a_{33} \cdot x_3(t)]$$

This function returns a vector with the value of:

$$\begin{aligned} & r_1 \cdot x_1(t) + x_1(t) \cdot [a_{11} \cdot x_1(t) + a_{12} \cdot x_2(t) + a_{13} \cdot x_3(t)] \\ & r_2 \cdot x_2(t) + x_2(t) \cdot [a_{21} \cdot x_1(t) + a_{22} \cdot x_2(t) + a_{23} \cdot x_3(t)] \\ & r_3 \cdot x_3(t) + x_3(t) \cdot [a_{31} \cdot x_1(t) + a_{32} \cdot x_2(t) + a_{33} \cdot x_3(t)] \end{aligned}$$

Value

Returns a vector with the value of the right side of the gLV equations.

Examples

```
cinit1<-c(x1<-0.7,x2<-0.2,x3<-0.1)
parms1= cbind(c(0.1,0.2,-0.1),c(-0.2,0.1,-0.1),c(0.3,0.2,0.3),c(0.1,0.22,0.2))
rxnrate(cinit1,parms1)
```

 Simulated

Gut microbiome simulated dataset

Description

Simulated dataset with 5 microbial taxa and 10 time points. Following the scheme given by Faust et al (2018), we generated the interaction matrix using the algorithm proposed by Klemm and Eguíluz (2002), and we generated the initial abundances using the Poisson distribution. With these two tools, we simulated the data using the generalized Lotka-Volterra structure. We carried out the simulation using the R package seqtime (Faust et al, 2018). Focusing on technical details, to generate the interaction matrix we set the clique size at 4, the diagonal values at -1, the interaction connectance at 0.04, the positive edge percentage at 64

Usage

```
data(Simulated)
```

Format

A data frame with 10 rows and 6 columns.

References

- K. Faust, F. Bauchinger, B. Laroche et al., “Signatures of ecological processes in microbial community time series”. *Microbiome*, vol. 6, no. 1, p. 120, 2018
- K. Klemm and V. M. Eguíluz, “Growing scale-free networks with small-world behavior”. *Physical Review*, vol. 65, no. 5, Article ID 057102, 2002.

 StudyingParam

Controlling quality of the convergence in BPBM

Description

This function controls that the value of the Rhat is between 0.9 and 1.1. In addition, it controls that the effective sample size is bigger than 100 and that the zero is not at the center of the credible interval (the interval between 2.5 and 97.5). We consider that the zero is in the center of the credible interval when the zero is between the 25 and the 75 quantile of the distribution formed by the limits of the credible interval.

Usage

```
StudyingParam(Sum, MCMC.CHAINS)
```

Arguments

Sum	Matrix with the summary of the "Estimating_BPBM". It is the output of the "Estimating_BPBM" adding "\$R2jagsOutput\$BUGSoutput\$summary".
MCMC.CHAINS	Matrix with the values of all the Markov chains for all parameters. It is the output of the "Estimating_BPBM" adding "\$SamplesAllChains".

Value

Returns a list with:

- Param.Summary: Matrix. The matrix Sum with a zero in the column Sum[, "mean"] when a parameter has the zero in the center of its credible interval.
- AllChainsJoined: Matrix. The matrix MCMC.CHAINS with a zero in all the iterations of the chain when a parameter has the zero in the center of its credible interval.

Examples

```
set.seed(314)
especie=t(gtools::rdirichlet(n=6, c(6,6,1,6,6)))
E=5
Tt=6
MatrizPBmodelo=rbind(c(1,1,1,1,1,1),c(-0.3,0.4,0.3,-0.7,-0.4,-0.6),c(0.3,0.5,-0.3,0.1,0.4,0.1))

est=Estimating_BPBM(especie,
                    Tt,
                    E,
                    MatrizPBmodelo,
                    nn.chain=3,
                    nn.burnin=1000,
                    nn.sample=5000,
                    nn.thin=10)

StudyingParam(est$R2jagsOutput$BUGSoutput$summary, est$SamplesAllChains)
```

TableBPBM

Obtaining a table with the SPBal information of the BPBM

Description

Returns a table with the percentage of variance that each SPBal has, the bacteria that goes in the numerator and denominator of the balance, the relationship between the group in the numerator and the denominator and the bacteria most influenced by this SPBal.

Usage

```
TableBPBM(
  NumSPBal,
  DemSPBal,
  PerVar,
  MatrizPBmodelo,
  Estimated.Param,
  BB = 0.55,
  names,
  E
)
```

Arguments

NumSPBal	List. Output of "ObtainigValueSPBal" function.List. The component i of the list has the number of the row of the matrix <i>especie</i> where the bacteria in the numerator of the selected principal balance i are placed.
DemSPBal	List. Output of "ObtainigValueSPBal" function.List. The component i of the list has the number of the row of the matrix <i>especie</i> where the bacteria in the denominator of the selected principal balance i are placed.
PerVar	Vector. Output of "ObtainigValueSPBal" function. The component of the vector i contains the percentage of variance of the SPBal with numerator NumSPBal[[i]] and denominator DemSPBal[[i]].
MatrizPBmodelo	Matrix. Output of "ObtainigValueSPBal" function. MatrixSPBal is the matrix that contains the covariates of the model. The first line es equal to 1 for all columns. The other rows contain the value of one SPBal at all time points. The selected principal balance of the row $i+1$ has at its numerator the bacteria placed in the rows NumSPBal[[i]] of the "especie". The selected principal balance of the row $i+1$ has at its denominator the bacteria placed in the rows DemSPBal[[i]] of the "especie".
Estimated.Param	Vector. Column "mean" of the output of StudyingParam function.
BB	The bacteria in the numerator and the denominator of the balance are considered similar if the mean of the SPBal is between $(-BB, BB)$.Default: 0.55.
names	Vector with the bacteria's names placed in the order in which appear in the rows of the matrices <i>especie</i> and <i>especiemodi</i> .
E	number of bacteria in the dataset.

Value

Returns the table written in latex

Examples

```
NumSPBal=list(c(3,4),3,2)
DemSPBal=list(1,5,4)
PerVar=c(41.37487, 21.08270, 19.16870)
```

```

MatrizPBmodelo=rbind(c(1.00000000, 1.00000000, 1.00000000, 1.00000000 , 1.00000000),
                     c(1.84449081, -1.3569851, -0.1388348, -0.5269079, -1.3288684),
                     c(0.27531685, 0.4741394, -1.9045554, -0.3581268, -0.4768543),
                     c( 0.07782991, 0.3492473, -0.7138882, 1.4332828, -0.7203295))
namesOr=c("Bact1", "Bact2", "Bact3", "Bact4", "Bact5")
Estimated.Param=c(0.5, 0.3, -0.2, 0.1)
E=5

```

```

TableBPBM(NumSPBal,
          DemSPBal,
          PerVar,
          MatrizPBmodelo,
          Estimated.Param,
          BB=0.55,
          namesOr,
          E)

```

TableFBM

Obtainig a table with the interpretable parameters

Description

This function returns a table with the interpretable parameters of the FBM model.

Usage

```
TableFBM(paramEstimadosFinal, names, E)
```

Arguments

paramEstimadosFinal

The estimate parameters, in the following order: a11,a12,a13, a21, a22,a23, ...a(D-1)1,a(D-1)2,a(D-1)3,tau. Where D is the number of bacterial species present in the matrix especie.

names

Vector of length D. The component i has the name of the bacteria i.

E

Number of bacteria available.

Details

$\mu_{it} = a_{i1} + a_{i2} \cdot \text{alr}(x_{i,(t-1)}) + a_{i3} \cdot \text{Balance}(x_{i,(t-1)})$ for $i = 1, \dots, D-1$ where D is the number of bacteria

Value

Returns a table written in latex format.

References

Creus-Martí, I., Moya, A., Santonja, F. J. (2021). A Dirichlet autoregressive model for the analysis of microbiota time-series data. *Complexity*, 2021, 1-16.

Examples

```
paramEstimadosFinal=c(1,2,3,1,2,3,1,2,3)
names=c("Bact1", "Bact2", "Bact3")
E=3

TableFBM(paramEstimadosFinal,names,E)
```

Table_alr_Dirich_glv *Obtainig a table with the interpretable parameters*

Description

This function returns a table with the interpretable parameters of the Dirich-gLV model.

Usage

```
Table_alr_Dirich_glv(Param.Estimates, especie, names, E)
```

Arguments

Param.Estimates

Vector with the estimates parameters. It is equal to `c(tau, as.vector(pam))` where:

- pam Matrix. Each row has the parameters of each bacteria. Following our example, pam has the parameters placed as follows:

r1	a11	a12
r2	a21	a22

- tau Number. Value of the tau parameter in the model

especie Matrix that contains at row *i* the bacterial taxa of bacteria *i* at all time points. The bacteria placed in the last row of this matrix is the one used as reference in the alr transformation that the model applies.

names Vector with the name of the bacteria in the same order than are present in the especie matrix.

E Number of bacteria available.

Details

In an example with three bacteria, the regression of this model is defined by

$$r_1 \cdot \log(x_1(t)/x_3(t)) + \log(x_1(t)/x_3(t)) \cdot [a_{11} \cdot \log(x_1(t)/x_3(t))(t) + a_{12} \cdot \log(x_2(t)/x_3(t))]$$

$$r_2 \cdot \log(x_2(t)/x_3(t)) + \log(x_2(t)/x_3(t)) \cdot [a_{21} \cdot \log(x_1(t)/x_3(t))(t) + a_{22} \cdot \log(x_2(t)/x_3(t))]$$

Value

Returns a table written in latex format with the matrix pam.

References

Creus-Martí, I. and Moya, A. and Santonja, F. J. (2018). A Statistical Model with a Lotka-Volterra Structure for Microbiota Data. Lucas Jodar, Juan Carlos Cortes and Luis Acedo, Modelling or engineering and human behavior 2018, Instituto Universitario de Matematica Multidisciplinar. ISBN: 978-84-09-07541-6

Examples

```
pam.ini=rbind(c(0.1,0.2,0.3),c(0.4,0.5,0.6))
paramEstimadosFinal=c(5, as.vector(pam.ini))
E=3
especie=cbind(c(0.2,0.4,0.4),c(0.1,0.1,0.8),c(0.5,0.1,0.4))
names=c("a","b","c")
```

```
Table_alr_Dirich_glv(paramEstimadosFinal,especie,names,E)
```

TauAndParameters_EstParmFunc_FBM

Obtaining the value of tau and the estimate value of the rest of the parameters

Description

This function estimates the parameters of the FBM model.

Usage

```
TauAndParameters_EstParmFunc_FBM(
  ttau = 30,
  ridge.final,
  Iter.EstParmFunc = 80,
  especie,
  EspecieMaxima,
```



```

    Tt,
    E,
    seed = NULL
)

```

Arguments

<code>ttau</code>	Number. We estimate de FBM model for the values of tau: 1, 2,..., ttau
<code>ridge.final</code>	Object of class "ridgelm". Values obtained with the ridge regression.
<code>Iter.EstParmFunc</code>	Number. Number of iterations. Default: 80 iterations.
<code>especie</code>	Matrix that contains at row <i>i</i> the bacterial taxa of bacteria <i>i</i> at all time points. The bacteria placed in the last row of the matrix will be used as reference in the alr transformation and will be at the denominator of the balance.
<code>EspecieMaxima</code>	Row in which the bacteria used as reference is in <code>especie</code> . This is the bacteria that is going to be at the denominator of the balance and at the denominator of the alr transformartion. As a result, in this function, <code>EspecieMaxima</code> must be equal to <code>E</code>
<code>Tt</code>	Number of time points available
<code>E</code>	Number. Number of bacteria available.
<code>seed</code>	Number. Set a seed. Default seed=NULL.

Details

We give to the parameter tau the value 1,2,...,ttau. We estimate the FBM model for all this values (using the function "Estimate_param_FBM") and we select the value of tau that minimizes the AIC. The regression of this model is defined by

$$\mu_{it} = a_{i1} + a_{i2} \cdot \text{alr}(x_{i,(t-1)}) + a_{i3} \cdot \text{Balance}(x_{i,(t-1)}) \text{ for } i = 1, \dots, D-1 \text{ where } D \text{ is the number of bacteria}$$

Value

Returns a list with:

- `EstimateParameters`: Vector with the estimated parameters, in the following order: `a11,a12,a13, a21, a22,a23, ...a(D-1)1,a(D-1)2,a(D-1)3,tau`. Where `D` is the number of bacterial species present in the matrix `especie`.
- `AIC Number`: Value of the AIC.
- `All.iter`: Matrix. Each row has the parameters obtained in each iteration. The parameters are in the columns written in the same order that they are written in `Param.Estimates`. In this matrix we must observe that in the last iterations the values has really similar or equal values, if not, we need to increase the value of `Iter.EstParmFunc`.

References

Creus-Martí, I., Moya, A., Santonja, F. J. (2021). A Dirichlet autoregressive model for the analysis of microbiota time-series data. *Complexity*, 2021, 1-16.

Examples

```

set.seed(123)
especie=t(gtools::rdirichlet(5,c(1,3,1)))
Tt=5
E=3
EspecieMaxima=3
ridge.final=ridgeregression(Tt,especie, E, EspecieMaxima)
ttau=10
Iter.EstParmFunc=10

TauAndParameters_EstParmFunc_FBM(ttau,ridge.final,Iter.EstParmFunc, especie,EspecieMaxima,Tt,E,714)

```

vector

*Alr of a bacteria***Description**

Writes a vector with the alr transformation of the bacteria *i* at time points $t=2, \dots, Tt$.

Usage

```
vector(i, especie, Tt, EspecieMaxima)
```

Arguments

<i>i</i>	Number. Position of the bacteria that we make the alr in the matrix <i>especie</i> . <i>i</i> must be different that <i>EspecieMaxima</i> .
<i>especie</i>	Matrix that contains at row <i>i</i> the bacterial taxa of bacteria <i>i</i> at all time points. The bacteria placed in the last row of the matrix will be used as reference in the alr transformation and will be at the denominator of the balance.
<i>Tt</i>	Number of time points available
<i>EspecieMaxima</i>	Row in which the bacteria used as reference is in <i>especie</i> . This is the bacteria that is going to be at the denominator of the balance and the denominator of the alr transformation. As a result, in this function, <i>EspecieMaxima</i> must be equal to <i>E</i>

Value

Returns a vector with the alr transformation of the bacteria *i* at time points $t=2, \dots, Tt$.

Examples

```

set.seed(123)
especie=t(gtools::rdirichlet(10,c(1,3,1,2,4)))
Tt=10
EspecieMaxima=5

```

```
i=2
vector(i, especie, Tt, EspecieMaxima)
```

ZeroData	<i>Zero replacement</i>
----------	-------------------------

Description

In this function the zeros are removed or replaced using functions of "zCompositions" package that can be used with longitudinal data (because they do not use the information of other rows to make the replacement).

Usage

```
ZeroData(DaTa, method = "multKM", seed = NULL)
```

Arguments

DaTa	data.frame. The first column contains the time point information (natural numbers 1,2,3...). The rest of the columns contain the relative abundance of each bacteria at the different time points. The values of each column must sum 1.
method	Character. <ul style="list-style-type: none"> • If method="multKM" - The replacement is carried out with the "multiplicative Kaplan-Meier smoothing spline replacement" (Palarea-Albaladejo and Martín-Fernandez, 2015). Default method. The zeros must be written with a 0. • If method="multRepl" - The replacement is carried out with the "multiplicative simple replacement" (Palarea-Albaladejo and Martín-Fernandez, 2015). The zeros must be written with a 0. • If method="nozeros" - The bacteria that contains zeros are removed. One column is added to the dataset called "Other".
seed	Number. Set a seed. Default seed=NULL.

Value

The dataset without zeros.

References

Palarea-Albaladejo J. and Martín-Fernandez JA. zCompositions – R package for multivariate imputation of left-censored data under a compositional approach. *Chemometrics and Intelligent Laboratory Systems* 2015; 143: 85-96.

Examples

```
set.seed(2)
dat=gtools::rdirichlet(6,c(1,2,3,1,2,3))
dat2=dat
dat2[2,1]=0
dat2[2,2]=dat[2,1]+dat[2,2]
dat2[4,3]=0
dat2[4,4]=dat[4,3]+dat[4,4]

X <- cbind( c(1:6) ,dat2)

Final=ZeroData(X,"multKM",1)
Final2=ZeroData(X,"multRepl",1)
```

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