Package ‘QFASA’

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Title  Quantitative Fatty Acid Signature Analysis
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Description  Accurate estimates of the diets of predators are required in many areas of ecology, but for many species current methods are imprecise, limited to the last meal, and often biased. The diversity of fatty acids and their patterns in organisms, coupled with the narrow limitations on their biosynthesis, properties of digestion in monogastric animals, and the prevalence of large storage reservoirs of lipid in many predators, led to the development of quantitative fatty acid signature analysis (QFASA) to study predator diets.

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AIT.dist

Returns the distance between two compositional vectors using Aitchison’s distance measure.

Usage

AIT.dist(x.1, x.2)

Arguments

x.1 compositional vector
x.2 compositional vector

References


AIT.more

Used to provide additional information on various model components evaluated at the optimal solution, i.e., using the QFASA diet estimates and Aitchison distance measure.

Description

Used to provide additional information on various model components evaluated at the optimal solution, i.e., using the QFASA diet estimates and Aitchison distance measure.

Usage

AIT.more(alpha, predator, prey.quantiles)
backward.elimination

Arguments

alpha  composition QFASA diet estimate.
predator  fatty acid signature of predator.
prey.quantiles  matrix of fatty acid signatures of prey. Each row contains an individual prey signature from a different species.

AIT.obj

Used in solnp() as the objective function to be minimized when Aitchison distance measure is chosen.

Description

Used in solnp() as the objective function to be minimized when Aitchison distance measure is chosen.

Usage

AIT.obj(alpha, predator, prey.quantiles)

Arguments

alpha  vector over which minimization takes place.
predator  fatty acid signature of predator.
prey.quantiles  matrix of fatty acid signatures of prey. Each row contains an individual prey signature from a different species.

backward.elimination

Returns diet estimates corresponding to a sample of predators based on a backward elimination algorithm that chooses the prey species to be included in the modelling.

Description

Returns diet estimates corresponding to a sample of predators based on a backward elimination algorithm that chooses the prey species to be included in the modelling.
backward.elimination

Usage

backward.elimination(
  pred.mat,
  prey.mat,
  cal.vec,
  FC,
  ext.fa,
  k = 2,
  cutoff = 0.1,
  silence = FALSE
)

Arguments

pred.mat  matrix containing the FA signatures of the predators, where each row corresponds to a predator and each column to a FA.

prey.mat  data frame containing the FA signatures of the prey, where each row corresponds to a single individual prey. The first column must index the prey group, while the remaining columns correspond to FAs.

cal.vec  numeric vector of calibration coefficients corresponding to the FAs contained in the modelling subset ext.fa. A vector of ones in the length of ext.fa may be used for modelling without calibration coefficients.

FC  numeric vector of the average lipid contents for each prey group, in the order of the alphabetized prey groups. vector of ones equal in length to the number of prey groups may be used for modelling without adjustment for fat content.

ext.fa  character vector containing the subset of FAs to be used in modelling.

k  scaling factor to be used in calculating the value of the information criterion (IC). The default value of 2 corresponds to the Akaike Information Criterion. For a sample of size n, k = log(n) corresponds to the Bayesian Information Criterion. As this factor is numeric, values corresponding to other IC may be used freely.

cutoff  numeric proportion to be used as the threshold for the candidacy for removal of a species in backward elimination. If initial diet estimates for any individual predator find a species to be present in proportions greater than this threshold, that species will not be considered for removal from the model. This reduces computation times and safeguards against the removal of species which may be present in the diets of few predators. All species are considered candidates for removal at a value of 1, while lower values are more conservative. The default value is 0.1.

silence  if true, additional information is printed. Default is false.

Details

The function uses a backward elimination algorithm and the simplified MLE method to choose the prey species to be included in the model and then returns the diet estimates corresponding to these species.
Value

A list with components:

Diet_Estimates A matrix of the diet estimates for each predator where each row corresponds to a predator and each column to a prey species. The estimates are expressed as proportions summing to one.

Selection_Order A data frame summarizing each step of the algorithm, giving the order of species removal and the corresponding IC values.

Selection_Tables A list containing a data frame for each step of the selection process, providing the IC values associated with removing any one candidate species at that step.

See Also

forward.selection()

Examples

## This example takes some time to run.
## Please uncomment code below to run.

#library(dplyr)
#library(compositions)
## Package data: FAs
#data(FAset)
#fa.set = as.vector(unlist(FAset))

## Package data: Prey
#data(preyFAs)
#prey.sub=(preyFAs[,4:(ncol(preyFAs))][fa.set]
#prey.sub=prey.sub/apply(prey.sub,1,sum)
#group=as.vector(preyFAs$Species)
#prey.sub = cbind(group,prey.sub)
#sort.preytype <- order(prey.sub[, 1])
#prey.matrix <- prey.sub[sort.preytype,]

## Package data: Predators
#data(predatorFAs)
#tombstone.info = predatorFAs[,1:4]
#predator.matrix = predatorFAs[,5:(ncol(predatorFAs))]
#npredators = nrow(predator.matrix)

## Package data: Fat content
#FC = preyFAs[,c(2,3)]
#FC = as.vector(tapply(FC$lipid,FC$Species,mean,na.rm=TRUE))

## Package data: Calibration coefficients
#data(CC)
#cal.vec = CC[,2]
bal.diet.data

Sample example of balanced repeatability diet estimates data with only two repeated measurements per predator.

Description
Sample example of balanced repeatability diet estimates data with only two repeated measurements per predator.

Usage
bal.diet.data

Format
A data frame with 100 predator diets (50 unique predators) and 13 variables:

Seal.ID  Predator (1 to 50)
Year     Either 1 or 2
capelin  estimated diet proportion
coho     estimated diet proportion
eulachon estimated diet proportion
herring  estimated diet proportion
mackerel estimated diet proportion
pilchard estimated diet proportion
pollock  estimated diet proportion
sandlance estimated diet proportion
squid    estimated diet proportion
surfsmelt_s estimated diet proportion
surfsmelt_lg estimated diet proportion
Fatty acid calibration coefficients.

Fatty acid calibration coefficients.

Called by create.d.mat() to compute the chi-square distance.

Called by create.d.mat() to compute the chi-square distance.
chisq.dist

Returns the distance between two compositional vectors using the chi-square distance.

Description

Returns the distance between two compositional vectors using the chi-square distance.

Usage

chisq.dist(x.1, x.2, gamma)

Arguments

- x.1: compositional vector
- x.2: compositional vector
- gamma: power transform taken to be 1.

References


comp.rep

Repeatability in Diet Estimates

Description

Computes a measure of repeatability for a sample of predators with repeated diet estimate measurements.

Usage

comp.rep(
  data,
  prey.database,
  fatcont.mat,
  dist.meas,
  ext.fa,
  B = 50,
  R = 100,
  CI = FALSE,
  alpha = 0.05,
gamma.QFASA = 1,
gamma.rho = 1
}

Arguments

data           data frame of diet estimates. First column must denote the predator and second column the second factor (e.g. year or season).
prey.database   prey data base that was used to compute the QFASA diet estimates in data. Will be used to generate pseudo predators.
fatcont.mat     data frame or matrix of length equal to the number of prey FA signatures in prey data base. First column is name of species and second column is lipid.
dist.meas       distance measure to use in p.QFASA.
ext.fa          subset of FAs to use.
B               number of pseudo predators samples to generate for bias calculation. Default is set to 50 because is slow to run.
R               number of bootstrap samples (i.e. R samples for each generated sample of pseudo predators). Default is set to 100 because it is slow to run.
CI              indicates if a confidence interval for rho is to be calculated. Default is FALSE since this is time consuming to obtain.
alpha           a (1-alpha/2)X100 percent confidence interval is calculated for rho if CI=TRUE.
gamma.QFASA     if dist.meas=3, gamma is required. Default is 1.
gamma.rho       value of gamma to be used to compute CS distance in repeatablity functions. Default is 1.

Value

Bias corrected measure of repeatability, estimate of the bias and (if CI=TRUE) a confidence interval for the true repeatability.

References

"Repeatability for Compositional Diet Estimates with Zeros". Contact Connie Stewart (cstewart@unb.ca).

Examples

## These examples take some time to run.
## Please uncomment code below to run them.

# data(preyFAs)
# data(FAset)

## Balanced Diet Data

#my.preybase <- preyFAs[,c(1,3)]
# my.preybase[,1] <- my.preybase[,1]/rowSums(my.preybase[,1])
# set.seed(10)

# comp.rep(data = bal.diet.data, prey.database=my.preybase, 
# fatcont.mat = as.data.frame(preyFAs[,c(2,3)]), dist.meas=2, 
# ext.fa = as.vector(unlist(FAset)))

## Unbalanced Diet Data

# my.preybase <- preyFAs[,c(1,3)]
# my.preybase[,1] <- my.preybase[,1]/rowSums(my.preybase[,1])

# set.seed(10)

# comp.rep(unbal.diet.data, my.preybase, as.data.frame(preyFAs[,c(2,3)])),2, 
# as.vector(unlist(FAset)))

---

**conf.meth**

*Confidence Intervals for Diet Proportions*

**Description**

Returns simultaneous confidence intervals for the diet of each species in the prey database.

**Usage**

```r
conf.meth(
    predator.mat, 
    prey.mat, 
    p.mat, 
    cal.mat = rep(1, length(ext.fa)), 
    dist.meas, 
    FC = rep(1, nrow(prey.mat)), 
    alpha = 0.05, 
    nprey = 30, 
    R.p = 1, 
    R.ps = 100, 
    R = 100, 
    R.bias = 100, 
    noise = 0, 
    ext.fa
)
```

**Arguments**

- `predator.mat`: matrix containing fatty acid signatures of the predators with fatty acids summing to one.
prey.mat  
prey database. A data frame with first column a Species label and other columns fatty acid proportions summing to one..

p.mat  
matrix of previously computed predator diet estimates needed for confidence interval calculation.

cal.mat  
matrix or vector of calibration coefficients of predators. Each COLUMN corresponds to a different predator. Default is a vector of ones. The number of fatty acids should be the same as the number of predator and prey fatty acids.

dist.meas  
distance measure to use for estimation: 1=KL, 2=AIT or 3=CS

FC  
vector of prey fat content, one for each individual in prey database. Note that this vector is passed to the gen.pseudo.seals which expects fat content values for individual prey samples while pseudo.seal and p.QFASA expect a species average. Default is a vector of ones.

alpha  
1-alpha is the family-wise or overall confidence level. Default is 0.05 for an overall confidence level of 0.95.

nprey  
number of prey to sample from the prey database when generating pseudo predators for the nuisance parameter estimation using original QFASA simulating code. Default is 30.

R.p  
number of times to re-sample data. Due to algorithm being slow, the default parameter is 1.

R.ps  
number of pseudo predators to generate when estimating nuisance parameters. Default is 100.

R  
number of bootstrap replicates to use when generating p-values for confidence interval estimation. Default is 100.

R.bias  
number of replicates for bias computation. Default is 100.

noise  
proportion of noise to include in the generation of pseudo predators using original QFASA simulating code.

ext.fa  
subset of fatty acids to be used. These should be the same as those in predator.mat, prey.mat and cal.mat.

Details

Intervals are biased corrected as recommended in Stewart, C. (2013). Intervals are slow to obtain, particularly if there are many prey types. See vignette on parallel execution to speed up calculations.

Value

Simultaneous (1-alpha)*100 zero-inflated beta distribution.

References

create.d.mat

Examples

```r
## Reducing prey database to three species so that code below will run more quickly.
## Please uncomment code to run.

#set.seed(1234)
## Fatty Acids
#data(FAset)
#fa.set = as.vector(unlist(FAset))

## Sample of Predators
#data(predatorFAs)
#predator.matrix = predatorFAs[, -c(1:4)]
#predator.matrix.ext = predatorFAs[,fa.set]
#predator.matrix.ext = predator.matrix.ext/rowSums(predator.matrix.ext)

# Prey Database
#prey.red =
#preyFAs[preyFAs$Species=="capelin"|preyFAs$Species=="herring"|preyFAs$Species=="sandlance",]
#prey.red = prey.red[-c(1,3)]
#prey.red.ext = prey.red[,c("Species",fa.set)]
#prey.red.ext[-,1] <- prey.red.ext[-,1]/rowSums(prey.red.ext[-,1])
#prey.red.ext.means = MEANmeth(prey.red.ext)

## Calibration Coefficients

#data(CC)
#cal.vec = CC[CC$FA %in% fa.set, 2]

#diet.est <- p.QFASA(predator.mat = predator.matrix.ext,
#    prey.mat = prey.red.ext.means,
#    cal.mat = cal.vec,
#    dist.meas = 2,
#    start.val = rep(1,nrow(prey.red.ext.means)),
#    ext.fa = fa.set)["Diet Estimates"]

## conf.meth needs the full prey matrix unlike in p.QFASA
#ci <- conf.meth(predator.mat = predator.matrix.ext, prey.mat = prey.red.ext, cal.mat = cal.vec,
#    p.mat = diet.est, dist.meas = 2, ext.fa = fa.set)
```

create.d.mat

Called by testfordiff.ind.boot.fun() to create a matrix of distances.

Description

Called by testfordiff.ind.boot.fun() to create a matrix of distances.

Usage

create.d.mat(Y.1, Y.2)
Arguments

- **Y.1** vector
- **Y.2** vector

---

CS.more

*Used to provide additional information on various model components evaluated at the optimal solution, i.e., using the QFASA diet estimates and chi-square distance measure.*

---

Description

Used to provide additional information on various model components evaluated at the optimal solution, i.e., using the QFASA diet estimates and chi-square distance measure.

Usage

```r
CS.more(alpha, predator, prey.quantiles, gamma)
```

Arguments

- **alpha** compositional QFASA diet estimate.
- **predator** fatty acid signature of predator.
- **prey.quantiles** matrix of fatty acid signatures of prey. Each row contains an individual prey signature from a different species.
- **gamma** power transform exponent (see `chisq.dist()`).

---

CS.obj

*Used in `solnp()` as the objective function to be minimized when chi-square distance measure is chosen. Unlike `AIT.obj()` and `KL.obj()`, does not require modifying zeros.*

---

Description

Used in `solnp()` as the objective function to be minimized when chi-square distance measure is chosen. Unlike `AIT.obj()` and `KL.obj()`, does not require modifying zeros.

Usage

```r
CS.obj(alpha, predator, prey.quantiles, gamma)
```
Arguments

alpha  vector over which minimization takes place.
predator  fatty acid signature of predator.
prey.quantiles  matrix of fatty acid signatures of prey. Each row contains an individual prey signature from a different species.
gamma  power transform exponent (see chisq.dist()).

Description

List of fatty acids used in sample prey and predator data sets, preyFAs and predatorFAs respectively.

Usage

FAset

Format

A data frame with 39 observations and 1 variable:

<table>
<thead>
<tr>
<th>FA</th>
<th>Fatty acid name</th>
</tr>
</thead>
</table>

forward.selection

Returns diet estimates corresponding to a sample of predators based on a forward selection algorithm that chooses the prey species to be included in the modelling.

Description

Returns diet estimates corresponding to a sample of predators based on a forward selection algorithm that chooses the prey species to be included in the modelling.
forward.selection

Usage

```r
forward.selection(
    pred.mat, 
    prey.mat, 
    cal.vec, 
    FC, 
    ext.fa, 
    k = 2, 
    min.spec = 5, 
    starting.spec = NULL, 
    silence = FALSE
)
```

Arguments

- `pred.mat` matrix containing the FA signatures of the predators, where each row corresponds to a predator and each column to a FA.
- `prey.mat` data frame containing the FA signatures of the prey, where each row corresponds to a single individual prey. The first column must index the prey group, while the remaining columns correspond to FAs.
- `cal.vec` numeric vector of calibration coefficients corresponding to the FAs contained in the modelling subset ext.fa. A vector of ones in the length of ext.fa may be used for modelling without calibration coefficients.
- `FC` numeric vector of the average lipid contents for each prey group, in the order of the alphabetized prey groups. vector of ones equal in length to the number of prey groups may be used for modelling without adjustment for fat content.
- `ext.fa` character vector containing the subset of FAs to be used in modelling.
- `k` scaling factor to be used in calculating the value of the information criterion (IC). The default value of 2 corresponds to the Akaike Information Criterion. For a sample of size n, k = log(n) corresponds to the Bayesian Information Criterion. As this factor is numeric, values corresponding to other IC may be used freely.
- `min.spec` optional integer value specifying the minimum final model size for forward selection. By default, forward selection will add species to the model until the value of the chosen IC ceases to improve. If this parameter is increased, forward selection will add the best available species up to the specified minimum model size before continuing with the default selection process.
- `starting.spec` optional character vector specifying the starting species for the forward selection algorithm. Where known, two or more species may be specified to ensure their inclusion in the final model, reducing computation times for the algorithm. The default is NULL.
- `silence` if true, additional information is printed. Default is false.

Details

The function uses a forward selection algorithm and the simplified MLE method to choose the prey species to be included in the model and then returns the diet estimates corresponding to these species.
Value

A list with components:

Diet_Estimates  A matrix of the diet estimates for each predator where each row corresponds to a predator and each column to a prey species. The estimates are expressed as proportions summing to one.

Selection_Order  A data frame summarizing each step of the algorithm, giving the order of species selection and the corresponding IC values.

Selection_Tables  A list containing a data frame for each step of the selection process, providing the IC values associated with adding any one candidate species at that step.

See Also

backward.elimination()

Examples

## This example takes some time to run.
## Please uncomment code below to run.

#library(dplyr)
library(compositions)
## Package data: FAs
data(FAset)
#fa.set = as.vector(unlist(FAset))

## Package data: Prey
#data(preyFAs)
#prey.sub=(preyFAs[,4:(ncol(preyFAs))][fa.set]
#prey.sub=prey.sub/apply(prey.sub,1,sum)
#group=as.vector(preyFAs$Species)
#prey.sub = cbind(group,prey.sub)
#sort.preytype <- order(prey.sub[, 1])
#prey.matrix <- prey.sub[sort.preytype,]

## Package data: Predators
#data(predatorFAs)
#tombstone.info = predatorFAs[,1:4]
#predator.matrix = predatorFAs[,5:(ncol(predatorFAs))]
#npredators = nrow(predator.matrix)

## Package data: Fat content
#FC = preyFAs[,c(2,3)]
#FC = as.vector(tapply(FC$lipid,FC$Species,mean,na.rm=TRUE))

## Package data: Calibration coefficients
#data(CC)
#cal.vec = CC[,2]
#cal.mat = replicate(npredators, cal.vec)
rownames(cal.mat) <- CC$FA
names(cal.vec) <- rownames(cal.mat)

## QFASA (KL)
sample.qfasa <- p.QFASA(predator.matrix, MEANmeth(prey.matrix), cal.mat,
dist.meas = 1, gamma=1, FC,
start.val = rep(1, nrow(MEANmeth(prey.matrix))), fa.set)

## Forward Selection
#sample.fs <- forward.selection(predator.matrix, prey.matrix, cal.vec, FC, fa.set,
#min.spec = 5, starting.spec = c("capelin", "herring"))
## Output
#fs.estimates <- sample.fs$'Diet Estimates'

---

**KL.dist**

*Returns the distance between two compositional vectors using Kullback-Leibler distance measure.*

**Description**

Returns the distance between two compositional vectors using Kullback-Leibler distance measure.

**Usage**

KL.dist(x.1, x.2)

**Arguments**

- **x.1**: compositional vector
- **x.2**: compositional vector

**References**


---

**KL.more**

*Used to provide additional information on various model components evaluated at the optimal solution, i.e., using the QFASA diet estimates and Kullback-Leibler distance measure.*

**Description**

Used to provide additional information on various model components evaluated at the optimal solution, i.e., using the QFASA diet estimates and Kullback-Leibler distance measure.
**Usage**

```r
KL.more(alpha, predator, prey.quantiles)
```

**Arguments**

- `alpha`: compositional QFASA diet estimate.
- `predator`: fatty acid signature of predator.
- `prey.quantiles`: matrix of fatty acid signatures of prey. Each row contains an individual prey signature from a different species.

---

**KL.obj**

*Used in `solnp()` as the objective function to be minimized when Kullback–Leibler distance measure is chosen.*

**Description**

Used in `solnp()` as the objective function to be minimized when Kullback–Leibler distance measure is chosen.

**Usage**

```r
KL.obj(alpha, predator, prey.quantiles)
```

**Arguments**

- `alpha`: vector over which minimization takes place.
- `predator`: fatty acid signature of predator.
- `prey.quantiles`: matrix of fatty acid signatures of prey. Each row contains an individual prey signature from a different species.

---

**MEANmeth**

*Returns the multivariate mean FA signature of each prey group entered into the QFASA model. Result can be passed to `prey.mat` in `p.QFASA()`.*

**Description**

Returns the multivariate mean FA signature of each prey group entered into the QFASA model. Result can be passed to `prey.mat` in `p.QFASA()`.

**Usage**

```r
MEANmeth(prey.mat)
```
Arguments

prey.mat  matrix containing the FA signatures of the prey. The first column indexes the prey group.

mean_geometric  Returns the geometric mean of a compositional vector

Description

Returns the geometric mean of a compositional vector

Usage

mean_geometric(x)

Arguments

x  compositional vector

p.MLE  Returns simplified MLE diet estimates corresponding to a sample of predators.

Description

Computes the diet estimate for each predator in pred.mat using the simplified MLE method, without the use of random effects.

Usage

p.MLE(pred.mat, prey.mat, cal.mat, FC, ext.fa)

Arguments

pred.mat  matrix containing the FA signatures of the predators.
prey.mat  matrix containing the FA signatures of the individual prey. The first column must index the prey group. prey.mat is the prey database.
cal.mat  matrix of calibration factors where the \(i\) th column is to be used with the \(i\) th predator. If modelling is to be done without calibration coefficients, simply pass a vector or matrix of ones.
FC  vector of fat content of length equal to the number of prey groups or species.
ext.fa  subset of fatty acids to be used to obtain diet estimates.
Details

The assumed model is similar to the MUFASA model but the random effects are replaced by the prey species’ sample means to speed up computations. Unlike \textit{p.MUFASA}, this function does not require integration and hence is much faster.

Value

A list with components:

\begin{itemize}
  \item \texttt{Diet\_Estimates} A matrix of the diet estimates for each predator where each row corresponds to a predator and the columns to prey species. The estimates are expressed as proportions summing to one.
  \item \texttt{Var\_Epsilon} Optimized values of error variance. See reference.
  \item \texttt{nll} Negative log likelihood values. As per \textit{solnp} documentation, \texttt{nll} is a "vector of function values during optimization with last one the value at the optimal".
\end{itemize}

References


Examples

\begin{verbatim}
## This example takes some time to run.
## Please uncomment the code below to run.

#library(dplyr)
#library(compositions)

## Fatty Acids
#data(FAset)
#ext.fa <- as.vector(unlist(FAset))

## Predators
#data(predatorFAs)
#pred.mat <- predatorFAs[, -c(1:4)]
#n.pred <- nrow(pred.mat)

## Prey
#data(preyFAs)
#prey.mat <- preyFAs[, -c(1,3)]

#FC = preyFAs[,c(2,3)]
#FC = as.vector(tapply(FC$lipid,FC$Species,mean,na.rm=TRUE))

## Calibration Coefficients
#data(CC)
#cal.vec = CC[,2]
\end{verbatim}
#cal.mat = replicate(n.pred, cal.vec)
#rownames(cal.mat) <- CC$FA

## Diet Estimates
#mle.est <- p.MLE(pred.mat, prey.mat, cal.mat, FC, ext.fa)
#mle.est$"Diet Estimates"

p.MUFASA

Returns MUFASA diet estimates corresponding to a sample of predators.

Description

Computes the diet estimate for each predator in `pred.mat` using MLE method.

Usage

p.MUFASA(pred.mat, prey.mat, cal.mat, FC, ext.fa)

Arguments

- `pred.mat`: matrix containing the FA signatures of the predators.
- `prey.mat`: matrix containing FA signatures from each prey group. The first column must index the prey group. `prey.mat` is the prey database.
- `cal.mat`: matrix of calibration factors where the \(i\)th column is to be used with the \(i\)th predator. If modelling is to be done without calibration coefficients, simply pass a vector or matrix of ones. `cal.mat` must contain names of FAs.
- `FC`: vector of fat content of length equal to the number of prey groups or species.
- `ext.fa`: subset of fatty acids to be used to obtain QFASA diet estimates.

Value

A list with components:

- `Diet_Estimates`: A matrix of the diet estimates for each predator where each row corresponds to a predator and the columns to prey species. The estimates are expressed as proportions summing to one.
- `nll`: Negative log likelihood values. As per `solnp` documentation, `nll` is "Vector of function values during optimization with last one the value at the optimal".
- `Var_Epsilon`: Optimized values of error variance. See reference.

References

See Also

`p.MLE()` for a simplified version of `p.MUFASA()` that is faster to run.

Examples

```r
## This example takes some time to run.
## Please uncomment code below to run.

#library(dplyr)
#library(compositions)
## Fatty Acids
#data(FAset)
#fa.set = as.vector(unlist(FAset))

## Predators
#data(predatorFAs)
#tombstone.info = predatorFAs[,1:4]
#predator.matrix = predatorFAs[,5:(ncol(predatorFAs))]
#npredators = nrow(predator.matrix)

## Prey
## Extracting a small number of species to speed up calculations for the example.
#data(preyFAs)
#prey.matrix = preyFAs[-c(1,3)]
#spec.red <-c("capelin", "herring", "mackerel", "pilchard", "sandlance")
#spec.red <- sort(spec.red)
#prey.red <- prey.matrix %>% filter(Species %in% spec.red)

## Fat content
#FC = preyFAs[,c(2,3)]
#FC = FC %>% arrange(Species)
#FC.vec = tapply(FC$lipid,FC$Species,mean,na.rm=TRUE)
#FC.red <- FC.vec[spec.red]

## Calibration Coefficients
#data(CC)
#cal.vec = CC[,2]
#cal.m = replicate(npredators, cal.vec)
#rownames(cal.m) <- CC$FA

#M <- p.MUFASA(predator.matrix, prey.red, cal.m, FC.red, fa.set)

## Diet Estimates
#M$Diet_Estimates
```

**p.QFASA**

Returns QFASA diet estimates corresponding to a sample of predators.
Description

Computes the diet estimate for each predator in `predator.mat` using either the Kullback-Leibler Distance (KL), the Aitchison Distance (AIT) or the Chi-Square Distance (CS).

Usage

```r
p.QFASA(
predator.mat,
prey.mat,
cal.mat,
dist.meas,
gamma = 1,
FC = rep(1, nrow(prey.mat)),
start.val = rep(0.99999, nrow(prey.mat)),
ext.fa
)
```

Arguments

- **predator.mat**: matrix containing the FA signatures of the predators.
- **prey.mat**: matrix containing a representative FA signature from each prey group (usually the mean). The first column must index the prey group. Note can use function `MEANmeth` to calculate the means.
- **cal.mat**: matrix of calibration factors where the \( i \)th column is to be used with the \( i \)th predator. If modelling is to be done without calibration coefficients, simply pass a vector or matrix of ones.
- **dist.meas**: distance measure to use for estimation: 1=KL, 2=AIT or 3=CS
- **gamma**: parameter required for calculations using CS distance (passed to CS.obj). Currently being set to 1.
- **FC**: vector of fat content of length equal to the number of prey groups or species.
- **start.val**: initial vector of parameters to be optimized
- **ext.fa**: subset of fatty acids to be used to obtain QFASA diet estimates.

Details

Before carrying out an analysis using QFASA, rows of prey database must be normalized to sum to one. See Example for code that extracts a subset of FAs and then normalizes the prey database signatures.

Value

A list with components:

- **Diet Estimates**: A matrix of the diet estimates for each predator where each row corresponds to a predator and the columns to prey species. The estimates are expressed as proportions summing to one.
Additional Measures

For each predator for which a diet estimate was obtained:

- **ModFAS**
  - the value of the modelled fatty acid. These are expressed as proportions summing to one.

- **DistCont**
  - The contribution of each fatty acid to the final minimized distance.

- **PropDistCont**
  - The contribution of each fatty acid to the final minimized distance as a proportion of the total.

- **MinDist**
  - The final minimized distance.

References


Examples

```r
## Fatty Acids
data(FAset)
fa.set = as.vector(unlist(FAset))

## Predators
data(predatorFAs)
tombstone.info = predatorFAs[,1:4]
predator.matrix = predatorFAs[,5:(ncol(predatorFAs))]
npredators = nrow(predator.matrix)

## Prey
data(preyFAs)
prey.sub=(preyFAs[,4:(ncol(preyFAs))])[fa.set]
prey.sub=prey.sub/apply(prey.sub,1,sum)
group=as.vector(preyFAs$Species)
prey.matrix=cbind(group,prey.sub)
prey.matrix=MEANmeth(prey.matrix)

## Fat Content
FC = preyFAs[,c(2,3)]
FC = as.vector(tapply(FC$lipid,FC$Species,mean,na.rm=TRUE))

## Calibration Coefficients
data(CC)
cal.vec = CC[,2]
cal.mat = replicate(npredators, cal.vec)

## Run QFASA
Q = p.QFASA(predator.matrix, prey.matrix, cal.mat, dist.meas = 1, gamma=1,
```
FC, start.val = rep(1, nrow(prey.matrix)), fa.set)

## Diet Estimates
DietEst = Q$'Diet Estimates'

### p.sim.QFASA

<table>
<thead>
<tr>
<th>p.sim.QFASA</th>
<th>Simultaneous estimation of diet composition and calibration coefficients</th>
</tr>
</thead>
</table>

**Description**

Computes the diet estimate for each predator in `pred.sig` as well as an overall estimate of the calibration coefficient vector.

**Usage**

```r
p.sim.QFASA(pred.sig, prey.mat, FC = rep(1, nrow(prey.mat)))
```

**Arguments**

- **pred.sig**: matrix containing the FA signatures of the predator
- **prey.mat**: matrix containing a representative FA signature from each prey group (usually the mean). The first column must index the prey group.
- **FC**: vector of fat content of length equal to the number of prey groups (or species)

**Details**

Starting values for the diet estimates are equal proportions and a vector of ones is used for the calibration coefficients.

**Value**

A list with components:

- **diet.est**: A matrix of the diet estimates for each predator where each row corresponds to a predator and the columns to prey species. The estimates are expressed as proportions summing to one.
- **cc.est**: Estimated vector of calibration coefficients

**References**

Examples

```r
## This example takes some time to run.
## Please uncomment code below to run.

## Fatty Acids
#data(FAset)
#fa.set = as.vector(unlist(FAset))

## Predators
#data(predatorFAs)
tombstone.info = predatorFAs[,1:4]
predator.matrix = predatorFAs[,5:(ncol(predatorFAs))]
npredators = nrow(predator.matrix)

## Need predator and prey to have same length

#predator.ext <- predator.matrix[fa.set]
#predator.ext <- predator.ext/rowSums(predator.ext)

## Prey
#data(preyFAs)
prey.sub=(preyFAs[,4:(ncol(preyFAs))])[fa.set]
prey.sub=prey.sub/apply(prey.sub,1,sum)
group=as.vector(preyFAs$Species)
prey.matrix=cbind(group,prey.sub)
prey.matrix=MEANmeth(prey.matrix)

## Fat Content
#FC = preyFAs[,c(2,3)]
#FC = as.vector(tapply(FC$lipid,FC$Species,mean,na.rm=TRUE))

#Q.sim <-p.sim.QFASA(predator.ext,prey.matrix,FC)
## Average Diet Estimate
#round(colMeans(Q.sim[[1]]),3)
## Calibration Coefficients
#Q.sim[[2]]
```

---

**p.SMUFASA**

*Simultaneous maximum unified fatty acid signature analysis*

**Description**

Returns SMUFASA calibration coefficient estimates and an average diet among a sample of predators.

**Usage**

`p.SMUFASA(pred.mat, prey.mat, FC, ext.fa)`
Arguments

pred.mat  matrix containing the FA signatures of the predators.
prey.mat  matrix containing a representative FA signature from each prey group (usually the mean). The first column must index the prey group.
FC        vector of fat content of length equal to the number of prey groups or species.
ext.fa     subset of fatty acids to be used to obtain estimates.

Details

Calibration coefficients (CCs) are not supplied but are instead estimated. While one overall diet is computed, the CCs can be used in p.QFASA or p.MUFASA to estimate individual diet estimates.

Value

A list with components:

Cal_Estimates  A vector of estimated calibration coefficients common to all predators. The \( k \)th value corresponds to the \( k \)th fatty acid. The estimates sum to the number of fatty acids.
Diet_Estimate  A vector of estimates of the average diet among the predators. The estimates are expressed as proportions summing to one.
Var_Epsilon    Optimized values of error variance.
nll            Negative log likelihood values. As per \textit{solnp} documentation, \textit{nll} is "Vector of function values during optimization with last one the value at the optimal".

Examples

## This example takes some time to run.
## Please uncomment code below to run.

#library(dplyr)
#library(compositions)
## Fatty Acids
#data(FAset)
#fa.set = as.vector(unlist(FAset))

## Predators
#data(predatorFAs)
#tombstone.info = predatorFAs[,1:4]
#predator.matrix = predatorFAs[,5:(ncol(predatorFAs))]
#npredators = nrow(predator.matrix)

## Prey
## Extracting a small number of species to speed up calculations for the example.
#data(preyFAs)
#prey.matrix = preyFAs[-c(1,3)]
#spec.red <-c("capelin", "herring", "mackerel", "pilchard", "sandlance")
#spec.red <- sort(spec.red)
#prey.red <- prey.matrix %>% filter(Species %in% spec.red)
## Fat content

```r
#FC = preyFAs[,c(2,3)]
#FC = FC %>% arrange(Species)
#FC.vec = tapply(FC$lipid,FC$Species,mean,na.rm=TRUE)
#FC.red <- FC.vec[spec.red]

#out <- p.SMUFASA(predator.matrix, prey.red, FC.red, fa.set)
#out$Cal_Estimates
```

---

**POOLVARmeth**

*Computes within species variance-covariance matrices on transformed scaled, along with a pooled estimate.*

---

**Description**

Computes within species variance-covariance matrices on transformed scaled, along with a pooled estimate.

**Usage**

```r
POOLVARmeth(prey.mat)
```

**Arguments**

- **prey.mat** matrix containing transformed FA signatures of the prey. Note that the first column indexes prey type.

**Value**

Returns the variance-covariance matrix of each prey type as well as a pooled estimate of the variance-covariance matrix.

---

**predatorFAs**

*Predator fatty acid signatures. Each predator signature is a row with fatty acid proportions in columns.*

---

**Description**

Fatty acid signatures are subsetted for the chosen fatty acid set and renormalized during the modelling so there is no need to subset and/or renormalize prior to running p.QFASA. However, make sure that the same fatty acids appear in the predator and prey files (if a FA appears in one but not the other the code will give you an error).
Usage

predatorFAs

Format

A data frame with 10 observations and 70 variables:

SampleCode  TODO
AnimalCode   TODO
SampleGroup  TODO
Biopsy       TODO
c12.0
c13.0
Iso14
c14.0
c14.1w9
c14.1w7
c14.1w5
Iso15
Anti15
c15.0
c15.1w8
c15.1w6
Iso16
c16.0
c16.1w11
c16.1w9
c16.1w7
c7Mec16.0
c16.1w5
c16.2w6
iso17
c16.2w4
c16.3w6
c17.0
c16.3w4
c17.1
c16.4w3
c16.4w1
c18.0
  c18.1w13
  c18.1w11
  c18.1w9
  c18.1w7
  c18.1w5
  c18.2d5.11
  c18.2w7
  c18.2w6
  c18.2w4
  c18.3w6
  c18.3w4
  c18.3w3
  c18.3w1
  c18.4w3
  c18.4w1
  c20.0
  c20.1w11
  c20.1w9
  c20.1w7
  c20.2w9
  c20.2w6
  c20.3w6
  c20.4w6
  c20.3w3
  c20.4w3
  c20.5w3
  c22.1w11
  c22.1w9
  c22.1w7
  c22.2w6
  c21.5w3
  c22.4w6
  c22.5w6
  c22.4w3
  c22.5w3
  c22.6w3
  c24.1w9
Details

Unlike the original QFASApack code the predator data can contain as much tombstone data in columns as you wish but the predator FA signatures must be extracted as a separate input in order to run in p.QFASA.

---

**prey.cluster**

*Produces a dendrogram using distances between the mean FA signatures of the prey types.*

---

**Description**

Performs a hierarchical cluster analysis of mean prey fatty acid signatures using function hclust.

**Usage**

```r
prey.cluster(prey.fa, method = "complete", dist.meas = 2)
```

**Arguments**

- `prey.fa` data frame of prey fatty acid signature samples. First column must be species used to group samples. Other columns are assumed to be fatty acid proportions.
- `method` the agglomeration method to be used. This should be one of the possible methods in `hclust` such as "single", "complete" or "average". Default is "complete".
- `dist.meas` distance measure to use for calculating dissimilarities: 1=KL, 2=AIT or 3=CS. Default is AIT.

**Value**

Plot (dendrogram)

**Examples**

```r
## Fatty Acids
data(FAset)
fa.set = as.vector(unlist(FAset))

## prey.cluster requires full prey database.
data(preyFAs)
prey.sub=(preyFAs[,4:(ncol(preyFAs))][fa.set]
prey.sub=prey.sub/apply(prey.sub,1,sum)
group=as.vector(preyFAs$Species)
prey.matrix=cbind(group,prey.sub)

prey.cluster(prey.matrix,method="average",dist.meas=3)
```
prey.on.prey

Each prey fatty acid signature is systematically removed from the supplied prey database and its QFASA diet estimate is obtained by treating the individual as a predator.

Description

Each prey fatty acid signature is systematically removed from the supplied prey database and its QFASA diet estimate is obtained by treating the individual as a predator.

Usage

prey.on.prey(preybase, dist.meas, gamma = 1)

Arguments

preybase first column is name of species and remaining columns are fatty acids.
dist.meas see help file for p.QFASA.
gamma see help file for p.QFASA.

Value

diet estimate

Examples

data(preyFAs)
my.preybase <- preyFAs[, -c(1,3)]

# Note: uncomment examples to run. CRAN tests fail because execution time > 5 seconds
# diets.out <- prey.on.prey(my.preybase, 2)
# round(MEANmeth(diets.out), 3)

preyFAs

Prey fatty acid signatures. Each prey signature is a row with fatty acid proportions in columns.

Description

The prey file should contain all of the individual fatty acid signatures of the prey and their lipid contents (where appropriate) - a matrix of the mean values for the FAs (prey.matrix) by the designated prey modelling group is then calculated using the MEANmeth function.
Usage

preyFAs

Format

A data frame with 302 observations and 70 variables:

Lab.Code  TODO
Species  TODO
lipid  TODO
c12.0
c13.0
Iso14
c14.0
c14.1w9
c14.1w7
c14.1w5
Iso15
Anti15
c15.0
c15.1w8
c15.1w6
Iso16
c16.0
c16.1w11
c16.1w9
c16.1w7
c7Me16.0
c16.1w5
c16.2w6
Iso17
c16.2w4
c16.3w6
c17.0
c16.3w4
c17.1
c16.3w1
c16.4w3
c16.4w1
c18.0
c18.1w13
c18.1w11
c18.1w9
c18.1w7
c18.1w5
c18.2d5.11
c18.2w7
c18.2w6
c18.2w4
c18.3w6
c18.3w4
c18.3w3
c18.3w1
c18.4w3
c18.4w1
c20.0
c20.1w11
c20.1w9
c20.1w7
c20.2w9
c20.2w6
c20.3w6
c20.4w6
c20.3w3
c20.4w3
c20.5w3
c22.1w11
c22.1w9
c22.1w7
c22.2w6
c21.5w3
c22.4w6
c22.5w6
c22.4w3
c22.5w3
c22.6w3
c24.1w9
Details

Like the predator .csv file you can have as many tombstone data columns as required but there must be at least one column that identifies the modelling group, in this case, Species.

Unlike the predator data, the prey data is not subsetted and renomalized during the modelling so the prey file needs to be subsetted for the desired fatty acid set and renormalized to sum to 1 prior to calculating the mean values.

The full FA set is extracted from the data frame (columns 4 onward), subsetted for the FA set in use and then renormalized over 1. The modelling group names (the "Species" column in this case) is then added back to the subsetted and renormalized data (as the first column) and the average values calculated using the MEANmeth function. Note that for the MEANmeth function to work the modelling group name must be in the first column.

---

pseudo.pred

Generate a pseudo predator by sampling with replacement from prey database.

Description

Generates a single pseudo predator by sampling with replacement from prey database. To generate a sample of pseudo predators, please refer to example code.

Usage

pseudo.pred(diet, preybase, cal.vec, fat.vec, preysize = 2)

Arguments

diet  the "true" or "desired" diet of the pseudo predator with prey species in alphabetical order (i.e.in the order of table(preyFAs[,2])). A compositional vector of proportions that sums to one with length equal to the number of prey species.

preybase prey database from which to generate the pseudo predator. First column must provide the species name.

cal.vec  vector of calibration coefficients whose length is the same as the number of fatty acids in prey database.

fat.vec  vector of fat content whose length is the same as the number of species.

preysize number of prey to sample from prey database. If preysize=1, then one prey is selected from each species. Otherwise, a sample of n_k signatures (where n_k is sample size for species k) is obtained by sampling with replacement.

Details

The default is to re-sample all of the prey signatures within each species (that is, preysize=2). Alternatively, one prey may be randomly selected from each species yielding potentially more variable pseudo-predators. For details on simulating realistic predators signatures, see Bromaghin, J. (2015) Simulating realistic predator signatures in quantitative fatty acid signature analysis, Ecological Informatics, 30, 68-71.
pseudo.pred.norm

Description

Generate a pseudo predator parametrically from multivariate normal distributions.

Usage

pseudo.pred.norm(mu.mat, sigma.pool, diet)
Arguments

- **mu.mat**: matrix where each row represents the mean transformed FA signature of each prey type.
- **sigma.pool**: pooled variance-covariance matrix of the transformed fatty acid signatures of prey types.
- **diet**: the "true" or "desired" diet of the pseudo predator with prey species in the same order as the rows of mu.mat. A compositional vector of proportions that sums to one with length equal to the number of prey species.

Details

Similar to `pseudo.pred` but instead generates the pseudo-predators parametrically by assuming ilr transformed FA signatures have a multivariate normal distribution.

Value

A simulated predator FA signature. See `pseudo.pred` for an example illustrating how to generate a sample of pseudo predators.

---

**QFASA**

*QFASA: A package for Quantitative Fatty Acid Signature Analysis*

---

Description

Accurate estimates of the diets of predators are required in many areas of ecology, but for many species current methods are imprecise, limited to the last meal, and often biased. The diversity of fatty acids and their patterns in organisms, coupled with the narrow limitations on their biosynthesis, properties of digestion in monogastric animals, and the prevalence of large storage reservoirs of lipid in many predators, led us to propose the use of quantitative fatty acid signature analysis (QFASA) to study predator diets.

---

**QFASA.const.eqn**

*Returns sum(alpha) and used in solnp().*

---

Usage

`QFASA.const.eqn(alpha, predator, prey.quantiles, gamma)`
split_prey

Arguments

- alpha: vector over which minimization takes place.
- predator: fatty acid signature of predator.
- prey.quantiles: matrix of fatty acid signatures of prey. Each row contains an individual prey signature from a different species.
- gamma: power transform exponent (see chisq.dist).

Description

1. simulation prey database
2. modelling prey database

Usage

split_prey(prey.mat)

Arguments

- prey.mat: matrix of individual prey fatty acid signatures where the first column denotes the prey type

Details

IF number of samples of a prey type <=5, then prey.mod AND prey.sim are duplicated instead of split.

IF number of samples of a prey type <=5, then prey.mod AND prey.sim are duplicated instead of split.
testfordiff.ind.boot  Called by testfordiff.ind.pval().

Description

Called by testfordiff.ind.pval().

Usage

testfordiff.ind.boot(data, ns1, R)

Arguments

data  sample of compositional data
ns1  sample size of compdata.1
R  number of bootstrap samples. default is 500.

testfordiff.ind.boot.fun  Called by testfordiff.ind.boot().

Description

Called by testfordiff.ind.boot().

Usage

testfordiff.ind.boot.fun(data, i, ns1, change.zero = 1e-05)

Arguments

data  sample of compositional data
i  row index
ns1  sample size of compdata.1
change.zero  tolerance
testfordiff.ind.pval Test for a difference between two independent samples of compositional data. Zeros of any type are allowed.

Description
Test for a difference between two independent samples of compositional data. Zeros of any type are allowed.

Usage
testfordiff.ind.pval(compdata.1, compdata.2, R = 500)

Arguments
- compdata.1 sample of compositional data.
- compdata.2 sample of compositional data.
- R number of bootstrap samples, default is 500.

Value
p-value obtained through a multivariate permutation test with test statistic based on chi-square distances.

References

Examples
```r
# Prey
data(preyFAs)

# Capelin FA sig
capelin.sig=preyFAs[preyFAs$Species=="capelin",4:(ncol(preyFAs))]
capelin.sig=capelin.sig/apply(capelin.sig,1,sum)

capelin.sig=as.matrix(capelin.sig)

# Sandlance FA sig
sandlance.sig=preyFAs[preyFAs$Species=="sandlance",4:(ncol(preyFAs))]
sandlance.sig=sandlance.sig/apply(sandlance.sig,1,sum)

# Note: uncomment examples to run. CRAN tests fail because execution time > 5 seconds
# testfordiff.ind.pval(as.matrix(capelin.sig),as.matrix(sandlance.sig))```
unbal.diet.data

Sample example of unbalanced repeatability diet estimates data with a max of two repeated measurements per predator.

Description

Sample example of unbalanced repeatability diet estimates data with a max of two repeated measurements per predator.

Usage

unbal.diet.data

Format

A data frame with 96 predator diets (50 unique predators) and 13 variables:

Seal.ID  Predator (1 to 50)
Year     Either 1 or 2
capelin  estimated diet proportion
coho     estimated diet proportion
eulachon  estimated diet proportion
herring   estimated diet proportion
mackerel  estimated diet proportion
pilchard  estimated diet proportion
pollock   estimated diet proportion
sandlance estimated diet proportion
squid     estimated diet proportion
surfsmelt_s estimated diet proportion
surfsmelt_lg estimated diet proportion
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