

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 us to propose the use of quantitative fatty acid signature analysis (QFASA) to study predator diets.

Depends R (>= 3.2)

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Encoding UTF-8

LazyData true

Imports stats, Rsolnp, boot, futile.logger, gamlss, gamlss.dist

RoxygenNote 6.1.0

VignetteBuilder rmarkdown, knitr

Suggests knitr, rmarkdown, testthat, plyr, gtools

BugReports <https://github.com/justinkammerman/QFASA/issues>

URL <https://CRAN.R-project.org/package=QFASA>

NeedsCompilation no

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AIT.dist	<i>Returns the distance between two compositional vectors using Aitchison's distance measure.</i>
----------	---

Description

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

Aitchison, J., (1992) On criteria for measures of compositional difference. *Mathematical Geology*, 24(4), pp.365-379.

Connie Stewart (2017) An approach to measure distance between compositional diet estimates containing essential zeros, *Journal of Applied Statistics*, 44:7, 1137-1152, DOI: 10.1080/02664763.2016.1193846

AIT.more	<i>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.</i>
----------	---

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)
```

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.

AIT.obj	<i>Used in solnp() as the objective function to be minimized when Aitchison distance measure is chosen.</i>
---------	---

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.

beta.meths.CI	<i>Returns individual confidence intervals and simultaneous confidence intervals based on the zero-inflated beta distribution (not bias corrected - see note below).</i>
---------------	--

Description

For details see: Stewart, C. (2013) Zero-Inflated Beta Distribution for Modeling the Proportions in Quantitative Fatty Acid Signature Analysis. Journal of Applied Statistics, 40(5), 985-992.

Usage

```
beta.meths.CI(predator.mat, prey.mat, cal.mat = rep(1, length(ext.fa)),
  dist.meas, noise = 0, nprey, R.p, R.ps, R, p.mat, alpha, FC = rep(1,
  nrow(prey.mat)), ext.fa)
```

Arguments

predator.mat	matrix containing the fatty acid signatures of the predators.
prey.mat	prey database. A dataframe with first column a Species label and other columns fatty acid proportions. Fatty acid proportions are compositional.
cal.mat	matrix of calibration coefficients of predators. Each column corresponds to a different predator. At least one calibration coefficient vector must be supplied.
dist.meas	distance measure to use for estimation: 1=KL, 2=AIT or 3=CS

noise	proportion of noise to include in the simulation.
nprey	number of prey to sample from the the prey database when generating pseudo-predators for the nuisance parameter estimation.
R.p	number of beta diet distributions to generate for the nuisance parameters.
R.ps	number of pseudo predators to generate when estimating nuisance parameters.
R	number of bootstrap replicates to use when generating p-values for confidence interval estimation.
p.mat	matrix of predator diet estimates for which we are trying to find confidence interavls.
alpha	confidence interval confidence level.
FC	vector of prey fat content. 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.
ext.fa	subset of fatty acids to be used to obtain QFASA diet estimates.

Details

Note:

- These intervals are biased and should be corrected using the output from [bias.all](#).
- `CI.L.1` and `CI.U.1` contain the simultaneous confidence intervals.
- Slow because of bisection and lots of repetition.

Value

Individual confidence intervals and simultaneous confidence intervals based on the zero-inflated beta distribution. These intervals are biased and should be corrected using the output from [bias.all](#). `ci.l.1` and `ci.u.1` contain the simultaneous confidence intervals.

References

Stewart, C. (2013) Zero-inflated beta distribution for modeling the proportions in quantitative fatty acid signature analysis. *Journal of Applied Statistics*, 40(5), 985-992.

Examples

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

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

## Prey
prey.sub = preyFAs[, fa.set]
```

```

prey.sub = prey.sub / apply(prex.sub, 1, sum)
group = as.vector(prexFAs$Species)
prey.matrix.full = cbind(group,prey.sub)
prey.matrix = MEANmeth(prex.matrix.full)

## Calibration Coefficients
data(CC)
cal.vec = CC[CC$FA %in% fa.set, 2]
cal.mat = replicate(npredators, cal.vec)

# Note: uncomment examples to run. CRAN tests fail because execution time > 5 seconds
# set.seed(1234)
# diet.est <- p.QFASA(predator.mat = predator.matrix,
#                     prey.mat = prey.matrix,
#                     cal.mat = cal.mat,
#                     dist.meas = 2,
#                     start.val = rep(1,nrow(prex.matrix)),
#                     ext.fa = fa.set)[['Diet Estimates']]
#
# ci = beta.meths.CI(predator.mat = predator.matrix,
#                   prey.mat = prey.matrix.full,
#                   cal.mat = cal.mat,
#                   dist.meas = 2,
#                   nprey = 10,
#                   R.p = 1,
#                   R.ps = 10, #
#                   R = 1,
#                   p.mat = diet.est,
#                   alpha = 0.05,
#                   ext.fa = fa.set)

```

bias.all	<i>Calculate bias correction for confidence intervals from beta.meths.CI.</i>
----------	---

Description

Calculate bias correction for confidence intervals from [beta.meths.CI](#).

Usage

```

bias.all(p.mat, prey.mat, cal.mat = rep(1, length(ext.fa)),
        fat.cont = rep(1, nrow(prex.mat)), R.bias, noise, nprey, specify.noise,
        dist.meas, ext.fa)

```

Arguments

p.mat	matrix containing the fatty acid signatures of the predators.
prex.mat	matrix containing a representative fatty acid signature

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.
fat.cont	prey fat content
R.bias	bootstrap replicates
noise	noise
nprey	number of prey
specify.noise	noise
dist.meas	distance measure
ext.fa	subset of FA's to use.

Value

Row 1 is Lambda CI, row 2 is Lambda skew, and row 3 is Beta CI

Examples

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

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

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

## Calibration Coefficients
data(CC)
cal.vec = CC[CC$FA %in% fa.set, 2]
cal.mat = replicate(npredators, cal.vec)

# Note: uncomment examples to run. CRAN tests fail because execution time > 5 seconds
# diet.est <- p.QFASA(predator.mat = predator.matrix,
#                    prey.mat = prey.matrix,
#                    cal.mat = cal.mat,
#                    dist.meas = 2,
#                    start.val = rep(1,nrow(prey.matrix)),
#                    ext.fa = fa.set)[['Diet Estimates']]
#
# bias <- bias.all(p.mat = diet.est,
#                prey.mat = prey.matrix.full,
#                cal.mat = cal.mat,
```

```
#           R.bias = 10,  
#           noise = 0,  
#           nprey = 50,  
#           dist.meas = 2,  
#           ext.fa = fa.set)
```

CC	<i>Fatty acid calibration coefficients.</i>
----	---

Description

Fatty acid calibration coefficients.

Usage

CC

Format

A data frame with 66 observations and 2 variables:

FA fatty acid names

CC calibration coefficient for corresponding fatty acid

chisq.CA	<i>Called by create.d.mat() to compute the chi-square distance.</i>
----------	---

Description

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

Usage

chisq.CA(x1, x2)

Arguments

x1 vector

x2 vector

chisq.dist	<i>Returns the distance between two compositional vectors using the chi-square distance.</i>
------------	--

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

Stewart, C., Iverson, S. and Field, C. (2014) Testing for a change in diet using fatty acid signatures. *Environmental and Ecological Statistics* 21, pp. 775-792.

Connie Stewart (2017) An approach to measure distance between compositional diet estimates containing essential zeros, *Journal of Applied Statistics*, 44:7, 1137-1152, DOI: 10.1080/02664763.2016.1193846

create.d.mat	<i>Called by testfordiff.ind.boot.fun() to create a matrix of distances.</i>
--------------	--

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	<i>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.</i>
---------	--

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

```
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 <code>chisq.dist()</code>).

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

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

```
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 <code>chisq.dist()</code>).

FAset	<i>List of fatty acids used in sample prey and predator data sets, preyFAs and predatorFAs respectively.</i>
-------	--

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:

FA Fatty acid name

KL.dist	<i>Returns the distance between two compositional vectors using Kullback–Leibler distance measure.</i>
---------	--

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

S.J. Iverson, C. Field, W.D. Bowen, and W. Blanchard (2004) Quantitative fatty acid signature analysis: A new method of estimating predator diets, *Ecological Monographs* 72, pp. 211-235.

KL.more	<i>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.</i>
---------	--

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

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

Description

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

Usage

```
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.

mean.geometric	<i>Returns the geometric mean of a compositional vector</i>
----------------	---

Description

Returns the geometric mean of a compositional vector

Usage

```
## S3 method for class 'geometric'
mean(x)
```

Arguments

x	compositional vector
---	----------------------

MEANmeth	<i>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().</i>
----------	---

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

```
MEANmeth(preymat)
```

Arguments

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

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

Description

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

Usage

```
p.QFASA(predator.mat, prey.mat, cal.mat, dist.meas, gamma = 1,
         FC = rep(1, nrow(pre.y.mat)), start.val = rep(0.99999,
         nrow(pre.y.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.
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
start.val	initial vector of parameters to be optimized
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.

Additional Measures

For each predator for which a diet estimate was obtained:

ModFAS	the value of the modelled fatty acid (i.e., after CCs have been applied and the fatty acids subsetting and renormalised over the designated fatty acid set). 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.

Examples

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

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

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

FC = prexFAs[,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)
```

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 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

This function performs a hierarchical cluster analysis of prey fatty acid signatures using a matrix of dissimilarities for the n objects being clustered. Initially, each object is assigned as its own cluster and then the algorithm proceeds iteratively, at each stage joining the two most similar clusters, until there is just a single cluster.

Description

This function performs a hierarchical cluster analysis of prey fatty acid signatures using a matrix of dissimilarities for the n objects being clustered. Initially, each object is assigned as its own cluster and then the algorithm proceeds iteratively, at each stage joining the two most similar clusters, until there is just a single cluster.

Usage

```
prey.cluster(pre.y.fa, method, FUN)
```

Arguments

pre.y.fa	data frame of prey fatty acid signature samples. Species column is 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 'single', 'complete', 'average', 'median', 'centroid'.
FUN	distance function

Value

an object of class hclust which describes the tree produced by the clustering process.

prey.on.prey	<i>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.</i>
--------------	---

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(preibase, dist.meas, gamma = 1)
```

Arguments

preibase	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(prexFAs)
my.preibase <- prexFAs[, -c(1,3)]

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

prexFAs	<i>Prey fatty acid signatures. Each prey signature is a row with fatty acid proportions in columns.</i>
---------	---

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 renormalized 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	<i>Generate a pseudo predator by sampling with replacement from prey database.</i>
-------------	--

Description

Note: if preysize=1, then one prey is selecting from each species. otherwise, a sample of size n_k (number of species k) is sampled with replacement.

Usage

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

Arguments

diet	compositional vector of proportions that sums to one. Length is equal to the number of prey species.
preybase	prey database with first column providing the species name.
cal.vec	vector of calibration coefficients.
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.

Value

a simulated predator FA signature

Examples

```
data(prexFAs)

# Note: uncomment examples to run. CRAN tests fail because execution time > 5 seconds
# p.mat <- matrix(rep(NA,100*11),nrow=100)
# for (i in 1: 100) {
#   my.seal <- pseudo.pred(rep(1/11,11),
```

```

#           preyFAs[,-c(1,3)],
#           rep(1,ncol(preyFAs[,-c(1,3)]-1),
#           rep(1,11))
#   p.mat[i,] <- p.QFASA(my.seal,
#           MEANmeth(preyFAs[,-c(1,3)]),
#           rep(1,length(my.seal)),
#           2,
#           ext.fa=colnames(preyFAs[,-c(1:3)])$`Diet Estimates`
# }
#
# Average diet estimate
# round(apply(p.mat,2,mean),3)

```

pseudo.seal

Generate a single pseudo predator FA signature

Description

THIS IS THE NEW pseudo.seal FUNCTION THAT ALLOWS 1) FAT CONTENT TO BE INCLUDED IN THE GENERATED SEALS AND 2) SOME SPECIES TO BE TRULY ZERO (THAT IS, "ZERO SPECIES" DO NOT HAVE TO BE INCLUDED IN THE "NOISE") NOTE: IT IS ASSUMED THAT SUM(DIET) IS 1-NOISE

Usage

```
pseudo.seal(prey.sim, diet, noise, nprey, cal, fat.cont, specify.noise)
```

Arguments

prey.sim	OUTPUT OF split.prey
diet	DIET COMPOSITION VECTOR (NOTE: THIS VECTOR SHOULD SUM TO 1-NOISE. THE NOISE WILL BE ADDED TO THE diet VECTOR.)
noise	AMOUNT OF NOISE
nprey	nprey TOTAL NUMBER OF PREY TO BE SAMPLED
cal	CALIBRATION FACTORS
fat.cont	VECTOR OF FAT CONTENT OF LENGTH=I (# OF SPECIES)
specify.noise	A BOOLEAN VECTOR WITH TRUES DENOTING SPECIES TO USE IN NOISE.

Value

seal.star SIMULATED SEAL FA SIGNATURE.

 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().

Description

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

Usage

```
QFASA.const.eqn(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).

 split.prey

Splits prey database into a simulation set (1/3) and a modelling set (2/3). Returns a list:

Description

1. simulation prey database 2. modelling prey database

Usage

```
## S3 method for class 'prey'
split(pre.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.

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.l
 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.l
 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, ns1, R = 500)
```

Arguments

compdata.1	sample of compositional data.
compdata.2	sample of compositional data.
ns1	sample size of compdata.1.
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

Stewart, C., Iverson, S. and Field, C. (2014) Testing for a change in diet using fatty acid signatures. *Environmental and Ecological Statistics* 21, pp. 775-792.

Examples

```
## Prey
data(preyFAs)

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

## 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),
#                      nrow(capelin.sig))
```

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