Package 'breakaway'

December 1, 2023

```
Title Species Richness Estimation and Modeling
Version 4.8.4
Date 2022-11-17
Description Understanding the drivers of microbial diversity is an important frontier of micro-
                 bial ecology, and investigating the diversity of samples from microbial ecosystems is a com-
                 mon step in any microbiome analysis. 'breakaway' is the premier package for statistical analy-
                 sis of microbial diversity. 'breakaway' implements the latest and greatest esti-
                 mates of species richness, de-
                 scribed in Willis and Bunge (2015) <doi:10.1111/biom.12332>, Willis et al. (2017) <doi:10.1111/rssc.12206>, and Willis and Bunge (2015) <doi:10.1111/rssc.12
                 monly used estimates, including the objective Bayes approach de-
                 scribed in Barger and Bunge (2010) <doi:10.1214/10-BA527>.
License GPL-2
BugReports https://github.com/adw96/breakaway/issues
LazyData true
RoxygenNote 7.2.3
Depends R (>= 3.5.0)
Imports ggplot2,
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                 lme4,
                 magrittr,
                 MASS,
                 phyloseq,
                 stats,
                 tibble,
                 utils
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                 knitr,
                 plyr,
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                 dplyr
VignetteBuilder knitr
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```

R topics documented:

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```

alpha_estimate

alpha_estimate

Description

Build objects of class alpha_estimate from their components. alpha_estimate() is a constructor method

Usage

```
alpha_estimate(
  estimate = NULL,
 error = NULL,
 estimand = NULL,
 name = NULL,
  interval = NULL,
  interval_type = NULL,
  type = NULL,
 model = NULL,
 warnings = NULL,
  frequentist = NULL,
 parametric = NULL,
 plot = NULL,
  reasonable = NULL,
 other = NULL,
)
```

Arguments

estimate The estimate The standard error in the estimate error What is the estimate trying to estimate? (richness, Shannon...) estimand name The name of the method interval An interval estimate interval_type Type of interval estimate TODO(Amy): Deprecate? type model What model is fit warnings Any warnings?

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frequentist Logical. Frequentist or Bayesian?

parametric Logical. Parametric or not?

plot A ggplot associated with the estimate reasonable Is the estimate likely to be reasonable?

other Any other relevant objects

... Any other objects

Value

An object of class alpha_estimate

alpha_estimates

alpha_estimates

Description

Build objects of class alpha_estimates from their components. alpha_estimates() is a constructor method

Usage

```
alpha_estimates(...)
```

Arguments

... Objects of class alpha_estimate, or a list of objects of class alpha_estimate

Value

An object of class alpha_estimates

apples

(Data) Frequency count table of soil microbes in an apples orchard.

Description

(Data) Frequency count table of soil microbes in an apples orchard.

Usage

apples

Format

A data frame with 88 rows and 2 variables:

index an index variable

frequency number of taxa that were observed with this frequency ...

betta 5

References

Willis, A. and Bunge, J. (2015). Estimating diversity via frequency ratios. *Biometrics*, **71**(4), 1042–1049. doi:10.1111/biom.12332

Walsh, F. et al. (2014). (2014). Restricted streptomycin use in apple orchards did not adversely alter the soil bacteria communities. *Frontiers in Microbiology* **4**, 383.

betta

Modelling total diversity with betta

Description

This function tests for heterogeneity of total diversity (observed plus unobserved) across multiple sites. It can account or test for fixed effects that may explain diversity. It returns the significance of the covariates in explaining diversity and a hypothesis test for heterogeneity.

Usage

```
betta(
  chats = NULL,
  ses,
  X = NULL,
  initial_est = NULL,
  formula = NULL,
  data = NULL,
  p.digits = 3
)
```

Arguments

chats	A vector of estimates of total diversity at different sampling locations. 'breakaway' estimates are suggested in the high-diversity case but not enforced.
ses	The standard errors in chats, the diversity estimates. This can either be a vector of standard errors (with the arguments chats and X), or the name of the variable in the dataframe data that contains the standard errors (with the arguments formula and data).
X	A numeric matrix of covariates. If not supplied, an intercept-only model will be fit. This is optional with the chats argument.
initial_est	(Optional) A vector of length 1 + ncol(X) giving the starting values for the likelihood maximisation search. The first element is the starting estimate for sigma^2_u, and the remaining elements are the starting elements for beta. Defaults to NULL, in which case the starting values outlined in the paper are used.
formula	A formula object of the form $y \ x group$. Required with the data argument.
data	A dataframe containing the response, response standard errors, covariates, and grouping variable. Required with the formula argument.
p.digits	(Optional) A number that specifies the number of digits to which p-values will be rounded. The default value is 3 digits.

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Value

table A coefficient table for the model parameters. The columns give the parameter

estimates, standard errors, and p-values, respectively. This model is only as effective as your diversity estimation procedure; for this reason please confirm that your estimates are appropriate and that your model is not misspecified. betta_pic

may be useful for this purpose.

cov Estimated covariance matrix of the parameter estimates.

ssq_u The estimate of the heterogeneity variance.

homogeneity The test statistic and p-value for the test of homogeneity.

global The test statistic and p-value for the test of model explanatory power.

blups The conditional expected values of the diversity estimates (conditional on the

random effects). The authors propose that if the practitioner believes that information from one diversity estimator may inform the others, then using the 'condfits' as estimators of total diversity rather than 'Chats' may reduce vari-

ance of diversity estimates by "sharing strength" across the samples.

blupses The estimated standard deviation (standard errors) in the blups.

loglikelihood The log likelihood of the fitted model.

aic The Akaike information criterion for the fitted model.

aicc The finite sample correction of the Akaike information criterion for the fitted

model.

r_squared_wls The weighted R^2 statistic, appropriate for heteroskedastic linear models.

function.args A list containing values initially passed to betta_random.

Note

Ecologists who are interested in the way species richness varies with covariate information often run a regression-type analysis on the observed diversity using their covariate information as predictors. However, in many settings (especially microbial), rare and unobserved taxa play a hugely important role in explaining the subtleties of the ecosystem, however, a regression analysis on the observed diversity level fails to account for these unobserved taxa. By predicting the total level of diversity (for example, via breakaway) and estimating the standard error in the estimate, one can take account of these unobserved, but important, taxa. In order to account for the estimated nature of the response, a mixed model approach is taken, whereby the varying levels of confidence in the estimates contributes to a diagonal but heteroscedastic covariance matrix. Given covariates constitute the fixed effects in the mixed model, and significance of the random effect term "sigsq_u" reflects heterogeneity in the sample, that is, variability that cannot be explained by only the covariates. The authors believe this to be the first attempt at modelling total diversity in a way that accounts for its estimated nature.

Author(s)

Amy Willis

References

Willis, A., Bunge, J., and Whitman, T. (2015). Inference for changes in biodiversity. *arXiv* preprint. Willis, A. and Bunge, J. (2015). Estimating diversity via frequency ratios. *Biometrics*.

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See Also

breakaway; breakaway_nof1; apples

Examples

8 betta_lincom

betta_lincom	Confidence intervals and testing for linear combinations of fixed effects estimated via betta() or betta_random()
--------------	---

Description

This function provides point estimates, standard errors, and equal-tailed confidence intervals for linear combinations of fixed effects estimated via betta() or betta_random(). A p-value for a Wald test of the null that the linear combination of effects is equal to zero (against a general alternative) is also returned.

Usage

```
betta_lincom(fitted_betta, linear_com, signif_cutoff = 0.05)
```

Arguments

fitted_betta	A fitted betta object – i.e., the output of either betta() or betta_random() – containing fixed effect estimates of interest.
linear_com	The linear combination of fixed effects for which a point estimate, confidence interval, and hypothesis test are to be produced.
signif_cutoff	The type-I significance threshold for confidence intervals. Defaults to 0.05.

Value

table

A table containing a point estimate, standard error, lower and upper confidence bounds, and a p-value for the linear combination of fixed effects specified in input. The p-value is generated via a two-sided Wald test of the null that the linear combination of fixed effects is equal to zero.

Author(s)

David Clausen

References

Willis, A., Bunge, J., and Whitman, T. (2015). Inference for changes in biodiversity. arXiv preprint.

See Also

betta;

betta_pic 9

Examples

betta_pic

function for plotting total diversity

Description

A simple plotting interface for comparing total diversity across samples or a covariate gradient.

Usage

```
betta_pic(
   y,
   se,
   x = 1:length(y),
   ylimu = NULL,
   myy = NULL,
   mymain = NULL,
   mycol = NULL,
   labs = NULL,
   mypch = NULL,
   myxlim = NULL)
```

Arguments

У	A vector of estimates of total diversity. Other parameter estimates are accessible; this method may be used for plotting any parameter estimates
se	The standard errors in 'y', the diversity (or other parameter's) estimates.
30	The standard errors in y, the diversity (or other parameter s) estimates.
X	A vector of covariates to form the x-coordinates of the intervals. If no argument
	is given, defaults to the order.
ylimu	The upper endpoint of the y-axis.
myy	Deprecated, for backwards compatibility
mymain	Deprecated, for backwards compatibility
mycol	Deprecated, for backwards compatibility
labs	Deprecated, for backwards compatibility
mypch	Deprecated, for backwards compatibility
myxlim	Deprecated, for backwards compatibility

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Value

A ggplot object.

Author(s)

Amy Willis

References

Willis, A., Bunge, J., and Whitman, T. (2015). Inference for changes in biodiversity. arXiv preprint.

See Also

betta

Examples

```
betta_pic(c(1552, 1500, 884), c(305, 675, 205), mymain = "Example title")
```

betta_random

modelling total diversity with random effects

Description

This function extends betta() to permit random effects modelling.

Usage

```
betta_random(
  chats = NULL,
  ses,
  X = NULL,
  groups = NULL,
  formula = NULL,
  data = NULL,
  p.digits = 3
)
```

Arguments

chats

A vector of estimates of total diversity at different sampling locations. Required with the groups argument, and optionally with the X argument.

ses

The standard errors in chats, the diversity estimates. This can either be a vector of standard errors (with the arguments chats and X), or the name of the variable in the dataframe data that contains the standard errors (with the arguments formula and data).

Χ

A numeric matrix of covariates corresponding to fixed effects. If not supplied, an intercept-only model will be fit. Optional with the chats and groups arguments.

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groups A categorical variable representing the random-effects groups that each of the

estimates belong to. Required with the chats argument and optionally with the

X argument.

formula A formula object of the form y x | group. Required with the data argument.

data A dataframe containing the response, response standard errors, covariates, and

grouping variable. Required with the formula argument.

p.digits (Optional) A number that specifies the number of digits to which p-values will

be rounded. The default value is 3 digits.

Value

table A coefficient table for the model parameters. The columns give the parameter

estimates, standard errors, and p-values, respectively. This model is only as effective as your diversity estimation procedure; for this reason please confirm that your estimates are appropriate and that your model is not misspecified. betta_pic

may be useful for this purpose.

cov Estimated covariance matrix of the parameter estimates.

ssq_u The estimate of the heterogeneity variance.

ssq_g Estimates of within-group variance. The estimate will be zero for groups with

only one observation.

homogeneity The test statistic and p-value for the test of homogeneity.

global The test statistic and p-value for the test of model explanatory power.

blups The conditional expected values of the diversity estimates (conditional on the

random effects). Estimates of variability for the random effects case are un-

available at this time; please contact the maintainer if needed.

loglikelihood The log likelihood of the fitted model.

aic The Akaike information criterion for the fitted model.

aicc The finite sample correction of the Akaike information criterion for the fitted

model.

function.args A list containing values initially passed to betta_random.

Author(s)

Amy Willis

References

Willis, A., Bunge, J., and Whitman, T. (2015). Inference for changes in biodiversity. arXiv preprint.

See Also

betta;

Examples

```
df <- data.frame(chats = c(2000, 3000, 4000, 3000),
ses = c(100, 200, 150, 180),
Cont_var = c(100, 150, 100, 50),
groups = c("a", "a", "a", "b"))</pre>
```

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```
# formula notation
betta_random(formula = chats ~ Cont_var| groups,
ses = ses,
   data = df)

# direct input
betta_random(c(2000, 3000, 4000, 3000), c(100, 200, 150, 180),
X = cbind(Int = 1, Cont_var = c(100, 150, 100, 50)),
groups = c("a", "a", "a", "b"))

## handles missing data
betta_random(c(2000, 3000, 4000, 3000), c(100, 200, 150, NA),
groups = c("a", NA,
   "b", "b"))
```

breakaway

Species richness estimation with breakaway

Description

breakaway is a wrapper for modern species richness estimation for modern datasets

Usage

```
breakaway(
  input_data,
  cutoff = NA,
  output = NULL,
  plot = NULL,
  answers = NULL,
  print = NULL,
  ...
)
```

Arguments

input_data	An input type that can be processed by convert()
cutoff	The maximum frequency count to use for model fitting
output	Deprecated; only for backwards compatibility
plot	Deprecated; only for backwards compatibility
answers	Deprecated; only for backwards compatibility
print	Deprecated; only for backwards compatibility
	Additional arguments will be ignored; this is for backward compatibility

Value

An object of class alpha_estimate

breakaway_nof1 13

Note

'breakaway' presents an estimator of species richness that is well-suited to the high-diversity/microbial setting. However, many microbial datasets display more diversity than the Kemp-type models can permit. In this case, the log-transformed WLRM diversity estimator of Rocchetti et. al. (2011) is returned. The authors' experience suggests that some datasets that require the log-transformed WLRM contain "false" diversity, that is, diversity attributable to sequencing errors (via an inflated singleton count). The authors encourage judicious use of diversity estimators when the dataset may contain these errors, and recommend the use of breakaway_nof1 as an exploratory tool in this case.

Author(s)

Amy Willis

References

Willis, A. and Bunge, J. (2015). Estimating diversity via frequency ratios. *Biometrics*, **71**(4), 1042–1049.

See Also

```
breakaway_nof1; kemp; apples
```

Examples

```
breakaway(apples)
breakaway(apples, plot = FALSE, output = FALSE, answers = TRUE)
```

breakaway_nof1

species richness estimation without singletons

Description

This function permits estimation of total diversity based on a sample frequency count table. Unlike breakaway, it does not require an input for the number of species observed once, making it an excellent exploratory tool for microbial ecologists who believe that their sample may contain spurious singletons. The underlying estimation procedure is similar to that of breakaway and is outlined in Willis & Bunge (2014). The diversity estimate, standard error, estimated model coefficients and plot of the fitted model are returned.

Usage

```
breakaway_nof1(
  input_data,
  output = NULL,
  plot = NULL,
  answers = NULL,
  print = NULL
)
```

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Arguments

input_data An input type that can be processed by convert()
output Deprecated; only for backwards compatibility
plot Deprecated; only for backwards compatibility
answers Deprecated; only for backwards compatibility
print Deprecated; only for backwards compatibility

Value

An object of class alpha_estimate

code A category representing algorithm behaviour. 'code=1' indicates no nonlinear

models converged and the transformed WLRM diversity estimate of Rocchetti et. al. (2011) is returned. 'code=2' indicates that the iteratively reweighted model converged and was returned. 'code=3' indicates that iterative reweighting did not converge but a model based on a simplified variance structure was returned (in this case, the variance of the frequency ratios is assumed to be proportional to the denominator frequency index). Please peruse your fitted model

before using your diversity estimate.

name The "name" of the selected model. The first integer represents the numerator

polynomial degree and the second integer represents the denominator polyno-

mial degree. See Willis & Bunge (2014) for details.

para Estimated model parameters and standard errors.

est The estimate of total (observed plus unobserved) diversity.

seest The standard error in the diversity estimate.

full The chosen nonlinear model for frequency ratios.

Note

It is common for microbial ecologists to believe that their dataset contains false diversity. This often arises because sequencing errors result in classifying already observed organisms as new organisms. 'breakaway_nof1' was developed as an exploratory tool in this case. Practitioners can run 'breakaway' on their dataset including the singletons, and 'breakaway_nof1' on their dataset excluding the singletons, and assess if the estimated levels of diversity are very different. Great disparity may provide evidence of an inflated singleton count, or at the very least, that 'breakaway' is especially sensitive to the number of rare species observed. Note that 'breakaway_nof1' may be less stable than 'breakaway' due to predicting based on a reduced dataset, and have greater standard errors.

Author(s)

Amy Willis

References

Willis, A. (2015). Species richness estimation with high diversity but spurious singletons. *arXiv*. Willis, A. and Bunge, J. (2015). Estimating diversity via frequency ratios. *Biometrics*.

See Also

breakaway; apples

Examples

```
breakaway_nof1(apples[-1, ])
breakaway_nof1(apples[-1, ], plot = FALSE, output = FALSE, answers = TRUE)
```

```
build_frequency_count_tables
```

Build frequency count tables from an OTU table

Description

Build frequency count tables from an OTU table

Usage

```
build_frequency_count_tables(the_table)
```

Arguments

the_table

An OTU table as a data frame or a matrix. Columns are the samples and rows give the taxa.

Value

A list of frequency count tables corresponding to the columns.

chao1

Chaol species richness estimator

Description

This function implements the Chao1 richness estimate, which is often mistakenly referred to as an index.

Usage

```
chao1(input_data, output = NULL, answers = NULL)
```

Arguments

input_data An input type that can be processed by convert() or a phyloseq object

output Deprecated; only for backwards compatibility answers Deprecated; only for backwards compatibility

Value

An object of class alpha_estimate, or alpha_estimates for phyloseq objects

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Note

The authors of this package strongly discourage the use of this estimator. It is only valid when you wish to assume that every taxa has equal probability of being observed. You don't really think that's possible, do you?

Author(s)

Amy Willis

Examples

```
chao1(apples)
```

chao1_bc

Bias-corrected Chao1 species richness estimator

Description

This function implements the bias-corrected Chao1 richness estimate.

Usage

```
chao1_bc(input_data, output = NULL, answers = NULL)
```

Arguments

input_data An input type that can be processed by convert() or a phyloseq object

output Deprecated; only for backwards compatibility answers Deprecated; only for backwards compatibility

Value

An object of class alpha_estimate, or alpha_estimates for phyloseq objects

Note

The authors of this package strongly discourage the use of this estimator. It is only valid when you wish to assume that every taxa has equal probability of being observed. You don't really think that's possible, do you?

Author(s)

Amy Willis

Examples

```
chao1_bc(apples)
```

chao_bunge 17

chao_bunge	Chao-Bunge species richness estimator
------------	---------------------------------------

Description

This function implements the species richness estimation procedure outlined in Chao & Bunge (2002).

Usage

```
chao_bunge(input_data, cutoff = 10, output = NULL, answers = NULL)
```

Arguments

input_data An input type that can be processed by convert() or a phyloseq object

cutoff The maximum frequency to use in fitting.

output Deprecated; only for backwards compatibility
answers Deprecated; only for backwards compatibility

Value

An object of class alpha_estimate, or alpha_estimates for phyloseq objects

Author(s)

Amy Willis

Examples

chao_bunge(apples)

chao_shen	The Chao-Shen estimate of Shannon diversi	ty
-----------	---	----

Description

The Chao-Shen estimate of Shannon diversity

Usage

```
chao_shen(input_data)
```

Arguments

input_data An input type that can be processed by convert()

Value

An object of class alpha_estimate

18 convert

check_format

Run some basic checks on a possible frequency count table

Description

Run some basic checks on a possible frequency count table

Usage

```
check_format(output_data)
```

Arguments

output_data A matrix to test

Value

A checked frequency count table

convert

convert between different inputs for alpha-diversity estimates

Description

Inputs slated for development include phyloseq and otu_table

Usage

```
convert(input_data)
```

Arguments

input_data

Supported types include filenames, data frames, matrices, vectors...

Value

Frequency count able

cutoff_wrap 19

cutoff_wrap	Find a cut-off for estimates relying on contiguous counts
-------------	---

Description

Find a cut-off for estimates relying on contiguous counts

Usage

```
cutoff_wrap(my_data, requested = NA)
```

Arguments

my_data Frequency count table requested The user-requested cutoff

Value

Cutoff value

F_test	Conduct F test of null hypothesis $LB = 0$ using output from betta() or betta_random()

Description

This function performs an F-test of a null hypothesis LB = 0 where B is a vector of p fixed effects returned by betta() or betta_random() and L is an m x p matrix with linearly independent rows.

Usage

```
F_test(fitted_betta, L, method = "bootstrap", nboot = 1000)
```

Arguments

fitted_betta A fitted betta object - i.e., the output of either betta() or betta_random() - con-

taining fixed effect estimates of interest.

An m x p matrix defining the null LB = 0. L must have full row rank.

method A character variable indicating which method should be used to estimate the

distribution of the test statistic under the null.

nboot Number of bootstrap samples to use if method = "bootstrap". Ignored if method

= "asymptotic".

Value

A list containing

pval The p-value

F_stat The calculated F statistic

boot_F A vector of bootstrapped F statistics if bootstrap has been used. Otherwise

NULL.

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Author(s)

David Clausen

References

Willis, A., Bunge, J., and Whitman, T. (2015). Inference for changes in biodiversity. arXiv preprint.

See Also

```
betta;
betta_random;
betta;
get_F_stat
```

Examples

get_F_stat

Calculate F statistic under null hypothesis LB = 0 using output from betta() or $betta_random()$

Description

This function calculates an F statistic for a test of null hypothesis LB = 0 (against an unrestricted alternative) where B is a vector of p fixed effects returned by betta() or betta_random() and L is an m x p matrix with linearly independent rows.

Usage

```
get_F_stat(fitted_betta, L)
```

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Arguments

 $fitted_betta \qquad A \ fitted \ betta \ object-i.e., the \ output \ of \ either \ betta() \ or \ betta_random()-con-i.e., the \ output \ of \ either \ betta() \ or \ betta_random()-con-i.e., the \ output \ of \ either \ betta() \ or \ betta_random()-con-i.e., the \ output \ of \ either \ betta() \ or \ betta_random()-con-i.e., the \ output \ of \ either \ betta() \ or \ betta_random()-con-i.e., the \ output \ of \ either \ betta() \ or \ betta_random()-con-i.e., the \ output \ of \ either \ betta() \ or \ betta_random()-con-i.e., the \ output \ of \ either \ betta() \ or \ betta_random()-con-i.e., the \ output \ of \ either \ betta() \ or \ betta_random()-con-i.e., the \ output \ of \ either \ betta()-con-i.e., the \ output \ of \ either \ betta()-con-i.e., the \ output \ of \ either \ betta()-con-i.e., the \ output \ of \ either \ betta()-con-i.e., the \ output \ of \ either \ betta()-con-i.e., the \ output \ of \ either \ betta()-con-i.e., the \ output \ of \ either \ betta()-con-i.e., the \ output \ of \ either \ betta()-con-i.e., the \ output \ of \ either \ betta()-con-i.e., the \ output \ of \ either \ betta()-con-i.e., the \ output \ of \ either \ output \ output$

taining fixed effect estimates of interest.

An m x p matrix defining the null LB = 0. L must have full row rank.

Value

A list containing

F_stat The calculated F statistic

good_turing

The Good-Turing estimate of species richness

Description

The Good-Turing estimate of species richness

Usage

```
good_turing(input_data)
```

Arguments

input_data

An input type that can be processed by convert() or a phyloseq object

Value

An object of class alpha_estimate, or alpha_estimates for phyloseq objects

hawaii

(Data) Frequency count table of soil microbes in Hawaii.

Description

(Data) Frequency count table of soil microbes in Hawaii.

Usage

hawaii

Format

A data frame with 198 rows and 2 variables:

index an index variable

frequency number of taxa that were observed with this frequency ...

References

Willis, A. and Bunge, J. (2015). Estimating diversity via frequency ratios. *Biometrics*, **71**(4), 1042–1049. doi:10.1111/biom.12332

22 kemp

kemp Species richness estimation with Kemp-type	models
---	--------

Description

This function implements the species richness estimation procedure outlined in Willis & Bunge (2015). The diversity estimate, standard error, estimated model coefficients, model details and plot of the fitted model are returned.

Usage

```
kemp(
  input_data,
  cutoff = NA,
  output = NULL,
  plot = NULL,
  answers = NULL,
  print = NULL,
  ...
)
```

Arguments

input_data An input type that can be processed by convert()

cutoff The maximum frequency count to use for model fitting

output Deprecated; only for backwards compatibility

plot Deprecated; only for backwards compatibility

answers Deprecated; only for backwards compatibility

print Deprecated; only for backwards compatibility

Additional arguments will be ignored; this is for backward compatibility

Value

An object of class alpha_estimate

code A category representing algorithm behaviour. 'code=1' indicates no nonlinear

models converged and the transformed WLRM diversity estimate of Rocchetti et. al. (2011) is returned. 'code=2' indicates that the iteratively reweighted model converged and was returned. 'code=3' indicates that iterative reweighting did not converge but a model based on a simplified variance structure was returned (in this case, the variance of the frequency ratios is assumed to be proportional to the denominator frequency index). Please peruse your fitted model

before using your diversity estimate.

name The "name" of the selected model. The first integer represents the numerator

polynomial degree and the second integer represents the denominator polynomial degree of the model for the frequency ratios. See Willis & Bunge (2015)

for details.

para Estimated model parameters and standard errors.

est The estimate of total (observed plus unobserved) diversity.

make_design_matrix 23

seest The standard error in the diversity estimate.

full The chosen nonlinear model for frequency ratios.

ci An asymmetric 95% confidence interval for diversity.

Author(s)

Amy Willis

References

Willis, A. and Bunge, J. (2015). Estimating diversity via frequency ratios. *Biometrics*, **71**(4), 1042–1049.

Rocchetti, I., Bunge, J. and Bohning, D. (2011). Population size estimation based upon ratios of recapture probabilities. *Annals of Applied Statistics*, **5**.

See Also

```
breakaway; breakaway_nof1; apples
```

Examples

```
kemp(apples)
kemp(apples, plot = FALSE, output = FALSE, answers = TRUE)
```

make_design_matrix

Make design matrix

Description

Make design matrix

Usage

```
make_design_matrix(phyloseq_object, variables)
```

Arguments

phyloseq_object

A phyloseq object

variables variable names

Value

A matrix object giving the design matrix from the desired variables.

```
{\sf make\_frequency\_count\_table}
```

Draw frequency count subtables from an OTU table

Description

Draw frequency count subtables from an OTU table

Usage

```
make_frequency_count_table(labels)
```

Arguments

labels

A vector of counts of the taxa; i.e. a vector giving the number of times each taxon was observed.

Value

A frequency count table.

```
objective_bayes_geometric
```

Estimate species richness with an objective Bayes method using a geometric model

Description

Estimate species richness with an objective Bayes method using a geometric model

Usage

```
objective_bayes_geometric(
  data,
  output = TRUE,
  plot = TRUE,
  answers = FALSE,
  tau = 10,
  burn.in = 100,
  iterations = 2500,
  Metropolis.stdev.N = 75,
  Metropolis.start.theta = 1,
  Metropolis.stdev.theta = 0.3
)
```

Arguments

 $\begin{tabular}{lll} data & $TODO(Kathryn)(Kathryn)$\\ output & $TODO(Kathryn)(Kathryn)$\\ plot & $TODO(Kathryn)(Kathryn)$\\ answers & $TODO(Kathryn)(Kathryn)$\\ \end{tabular}$

 $\begin{array}{ll} \text{tau} & & TODO(Kathryn) \\ \\ \text{burn.in} & & TODO(Kathryn) \\ \\ \text{iterations} & & TODO(Kathryn) \\ \end{array}$

Metropolis.stdev.N

TODO(Kathryn)

Metropolis.start.theta

TODO(Kathryn)

Metropolis.stdev.theta

TODO(Kathryn)

Value

A list of results, including

est the median of estimates of N

,

ci a confidence interval for N

,

mean the mean of estimates of N

,

semeanest the standard error of mean estimates

,

dic the DIC of the model

,

fits fitted values

, and

diagnostics model diagonstics

.

```
objective_bayes_mixedgeo
```

Objective Bayes species richness estimate with the mixed-geometric model

Description

Objective Bayes species richness estimate with the mixed-geometric model

Usage

```
objective_bayes_mixedgeo(
   data,
   output = TRUE,
   plot = TRUE,
   answers = FALSE,
   tau = 10,
   burn.in = 100,
   iterations = 2500,
   Metropolis.stdev.N = 100,
   Metropolis.start.T1 = 1,
   Metropolis.start.T2 = 3,
   Metropolis.stdev.T2 = 2,
   bars = 3
)
```

Arguments

```
data
               TODO(Kathryn)
               TODO(Kathryn)
output
plot
               TODO(Kathryn)
               TODO(Kathryn)
answers
               TODO(Kathryn)
tau
burn.in
               TODO(Kathryn)
iterations
               TODO(Kathryn)
Metropolis.stdev.N
               TODO(Kathryn)
Metropolis.start.T1
               TODO(Kathryn)
Metropolis.stdev.T1
               TODO(Kathryn)
Metropolis.start.T2
               TODO(Kathryn)
Metropolis.stdev.T2
               TODO(Kathryn)
bars
               TODO(Kathryn)
```

objective_bayes_negbin 27

Value

A list of results, including

est the median of estimates of N
,
ci a confidence interval for N
,
mean the mean of estimates of N
,
semeanest the standard error of mean estimates
,
dic the DIC of the model
,
fits fitted values
, and
diagnostics model diagonstics

objective_bayes_negbin

Objective Bayes species richness estimate with the Negative Binomial model

Description

Objective Bayes species richness estimate with the Negative Binomial model

Usage

```
objective_bayes_negbin(
  data,
  output = TRUE,
  plot = TRUE,
  answers = FALSE,
  tau = 10,
  burn.in = 1000,
  iterations = 5000,
  Metropolis.stdev.N = 100,
  Metropolis.start.T1 = -0.8,
  Metropolis.start.T2 = 0.8,
  Metropolis.stdev.T2 = 0.01,
  bars = 5
)
```

Arguments

data TODO(Kathryn) TODO(Kathryn) output plot TODO(Kathryn) TODO(Kathryn) answers TODO(Kathryn) tau TODO(Kathryn) burn.in iterationsTODO(Kathryn) Metropolis.stdev.N TODO(Kathryn) Metropolis.start.T1 TODO(Kathryn) Metropolis.stdev.T1 TODO(Kathryn) Metropolis.start.T2 TODO(Kathryn) Metropolis.stdev.T2 TODO(Kathryn)

Value

bars

A list of results, including

est the median of estimates of N

TODO(Kathryn)

,

ci a confidence interval for N

,

mean the mean of estimates of N

,

semeanest the standard error of mean estimates

,

dic the DIC of the model

,

fits fitted values

, and

diagnostics model diagonstics

.

```
objective_bayes_poisson
```

Objective Bayes species richness estimate with the Poisson model

Description

Objective Bayes species richness estimate with the Poisson model

Usage

```
objective_bayes_poisson(
  data,
  output = TRUE,
  plot = TRUE,
  answers = FALSE,
  tau = 10,
  burn.in = 100,
  iterations = 2500,
  Metropolis.stdev.N = 75,
  Metropolis.start.lambda = 1,
  Metropolis.stdev.lambda = 0.3,
  bars = 5
)
```

Arguments

```
TODO(Kathryn)
data
output
               TODO(Kathryn)
               TODO(Kathryn)
plot
               TODO(Kathryn)
answers
               TODO(Kathryn)
tau
burn.in
               TODO(Kathryn)
iterations
               TODO(Kathryn)
Metropolis.stdev.N
               TODO(Kathryn)
Metropolis.start.lambda
               TODO(Kathryn)
Metropolis.stdev.lambda
               TODO(Kathryn)
               TODO(Kathryn)
bars
```

Value

```
A list of results, including
```

```
est the median of estimates of N , \label{eq:star} \mbox{$\rm ci$} \qquad \mbox{$\rm a$ confidence interval for N}
```

pasolli_et_al

,

mean the mean of estimates of N

,

semeanest the standard error of mean estimates

,

dic the DIC of the model

,

fits fitted values

, and

diagnostics model diagonstics

.

pasolli_et_al

 $(Data)\ Data\ frame\ of\ covariate\ information\ about\ pasolli_et_al.$

Description

(Data) Data frame of covariate information about pasolli_et_al.

Usage

```
pasolli_et_al
```

Format

A data frame with 4930 rows and 9 variables:

SGB.ID sample ID

Average Abundance average abundance in the sample

std standard deviation

q1 first quartile

MedianAbundance median abundance

q3 third quartile

min minimum

max maximum

#.Samples number of samples ...

physeq_wrap 31

physeq_wrap

Wrapper for phyloseq objects

Description

Wrapper for phyloseq objects

Usage

```
physeq_wrap(fn, physeq, ...)
```

Arguments

fn alpha diversity estimator function with breakaway to be applied to physeq
physeq A phyloseq object, or an object of class otu_table
... Additional arguments for fn

Value

Object of class alpha_estimates

Description

Plot function for alpha_estimates class

Usage

```
## S3 method for class 'alpha_estimates'
plot(
    x,
    physeq = NULL,
    measure = NULL,
    color = NULL,
    shape = NULL,
    title = NULL,
    trim_plot = FALSE,
    ...
)
```

32 poisson_model

Arguments

Object of class alpha_estimates. Х (Optional). Default NULL. Required object of class phyloseq if including a physeq sample_data variable for color or shape. measure (Optional). If there are multiple richness measures included in x, this can be set to the the desired measure to be plotted. Defaults to the measure of the first alpha diversity estimate. (Optional). Default NULL. The sample variable to map to different colors. Can color be a single character string of the variable name in sample_data or a custom supplied vector with length equal to the number of samples. (Optional). Default NULL. The sample variable to map to different shapes. Can shape be a single character string of the variable name in sample_data or a custom supplied vector with length equal to the number of samples. (Optional). Default NULL. Character string. The main title for the graphic. title (Optional). Default FALSE. Boolean indicator for whether you want the plot to trim_plot include the full confidence intervals. See details . . .

Details

... does not currently have any implemented options. Optional arguments currently include "trim_plot", a Optional

Value

A ggplot object.

Examples

library(phyloseq)
data(GlobalPatterns)
alphas <- breakaway(GlobalPatterns)
plot(alphas)</pre>

Description

A model to estimate the number of missing taxa under a Poisson Model

Usage

```
poisson_model(input_data, cutoff = 10)
```

Arguments

input_data A frequency count table

cutoff The largest frequency to use for predicting f0. Defaults to 10.

poisson_model_nof1 33

Value

An object of class alpha_estimate.

poisson_model_nof1

Poisson Model Nof 1

Description

A model to estimate the number of missing taxa under a zero- and one-truncated Poisson Model

Usage

```
poisson_model_nof1(input_data, cutoff = 10)
```

Arguments

input_data A frequency count table

cutoff The largest frequency to use for predicting f0 and f1. Defaults to 10.

Value

An object of class alpha_estimate.

proportions_instead

OTU table to relative abundances

Description

OTU table to relative abundances

Usage

```
proportions_instead(the_table)
```

Arguments

Value

A proportion table or vector.

34 rztnbinomtable

rnbinomtable

Negative binomially distributed frequency count tables.

Description

Simulate a frequency count table based on a negative binomial model. Zero-truncated, obviously.

Usage

```
rnbinomtable(C, size, probability)
```

Arguments

C species richness

size size parameter for the negative binomial distribution

probability probability parameter for the negative binomial distribution

Value

A simulated frequency count table.

Author(s)

Amy Willis

rztnbinomtable

beta version: Zero-truncated negative binomially distributed frequency count tables.

Description

Simulate a frequency count table based on a negative binomial model. Zero-truncated, obviously.

Usage

```
rztnbinomtable(C, size, probability)
```

Arguments

C species richness

size size parameter for the negative binomial distribution

probability probability parameter for the negative binomial distribution

Value

A simulated frequency count table.

Author(s)

Amy Willis

```
sample_inverse_simpson
```

Plug-in Inverse Simpson diversity

Description

This function implements the plug-in Inverse Simpson diversity

Usage

```
sample_inverse_simpson(input_data)
```

Arguments

input_data

An input type that can be processed by convert() or a phyloseq object

Value

An object of class alpha_estimate, or alpha_estimates for phyloseq objects

Examples

```
sample_inverse_simpson(apples)
```

sample_richness

Sample richness estimator

Description

This function implements the sample richness estimate, which is the number of non-zero taxa per sample.

Usage

```
sample_richness(input_data)
```

Arguments

input_data

An input type that can be processed by convert() or a phyloseq object

Value

An object of class alpha_estimate, or alpha_estimates for phyloseq objects

Examples

```
sample_richness(apples)
```

36 sample_shannon_e

sample_shannon

Plug-in Shannon diversity

Description

This function implements the plug-in Shannon diversity

Usage

```
sample_shannon(input_data)
```

Arguments

input_data

An input type that can be processed by convert() or a phyloseq object

Value

An object of class alpha_estimate, or alpha_estimates for phyloseq objects

Examples

```
sample_shannon(apples)
```

sample_shannon_e

Plug-in Shannon's E ("Equitability")

Description

This function implements the plug-in Shannon's E

Usage

```
sample_shannon_e(input_data)
```

Arguments

input_data

An input type that can be processed by convert() or a phyloseq object

Value

An object of class alpha_estimate, or alpha_estimates for phyloseq objects

Examples

```
sample_shannon_e(apples)
```

sample_simpson 37

sample_simpson

Plug-in Simpson diversity

Description

This function implements the plug-in Simpson diversity

Usage

```
sample_simpson(input_data)
```

Arguments

input_data

An input type that can be processed by convert() or a phyloseq object

Value

An object of class alpha_estimate, or alpha_estimates for phyloseq objects

Examples

```
sample_simpson(apples)
```

sample_size_estimate

Estimate the sample size needed to do an unpaired one-way test using betta

Description

Estimate the sample size needed to do an unpaired one-way test using betta

Usage

```
sample_size_estimate(
  control_group_est,
  se_est,
  diff = 5,
  alpha = 0.05,
  prop = 0.8,
  samples = 20,
  precision = 5
)
```

38 sample_size_figure

Arguments

control_group_est

An estimate of the alpha diversity parameter for the control group

se_est An estimate of the (common) standard deviation

diff An estimate of the difference between the control and non-control groups

alpha Minimum significance level desired

prop Desired power

samples Number of bootstrap resamples used to estimate the sample size. Increase for a

more accurate estimate.

precision How much to increment the sample size as we try to increase the power

Value

An estimate of the necessary sample size and some details

sample_size_figure

Plot the power obtained with sample size

Description

Plot the power obtained with sample size

Usage

```
sample_size_figure(control_group_est, se_est, diff = 5, samples = 20)
```

Arguments

control_group_est

An estimate of the alpha diversity parameter for the control group

se_est An estimate of the (common) standard deviation

diff An estimate of the difference between the control and non-control groups

samples Number of bootstrap resamples used to estimate the sample size. Increase for a

more accurate estimate.

Value

A plot of the power with the sample size

simulate_betta 39

simulate_betta

Simulate from a fitted betta model

Description

Simulate from a fitted betta model

Usage

```
simulate_betta(fitted_betta, nsim)
```

Arguments

fitted_betta A fitted betta object

nsim Number of times to simulate

Value

A list of length nsim, each element of which is a vector of simulated Y-values under the fitted betta model

 $simulate_betta_random$ Simulate from a fitted betta_random model

Description

Simulate from a fitted betta_random model

Usage

```
simulate_betta_random(fitted_betta, nsim)
```

Arguments

fitted_betta A fitted betta_random object
nsim Number of times to simulate

Value

A list of length nsim, each element of which is a vector of simulated Y-values under the fitted betta model

40 test_submodel

soil_phylo

(Data) Data frame of soil data from whitman_et_al.

Description

A phyloseq object with an OTU table and sample data from a soil microbiome study.

Usage

soil_phylo

Format

A phyloseq-class experiment-level object with an OTU table and sample data.

otu_table OTU table with 7,770 taxa and 119 samples

tax_table taxonomy table

sam_data sample data with the following covariates:

- Plants, values 0 and 1. Index for different plants
- Day, values 0 (initial sampling point), 1 (12 days after treatment additions), and 2 (82 days after treatment additions). Index for different days of measurement
- Amdmt, values 0 (no additions), 1 (biochar additions), and 2 (fresh biomass additions). Index for different soil additives.
- DayAmdmt, values 00, 01, 02, 10, 11, 12, 20, 21, and 22. A single index for the combination of Day and Amdmt with Day as the first digit and Amdmt as the second digit.
- ID, values A, B, C, D, and F. Index for different soil plots.

• • •

References

Whitman, T., Pepe-Ranney, C., Enders, A., Koechli, C., Campbell, A., Buckley, D. H., Lehmann, J. (2016). *Dynamics of microbial community composi-tion and soil organic carbon mineralization in soil following addition of pyrogenic and fresh organic matter*. The ISME journal, 10(12):2918. <doi: 10.1038/ismej.2016.68>.

test_submodel

Conduct F test of null hypothesis LB = 0 using output from betta() or betta_random()

Description

This function performs an F-test of a null hypothesis LB = 0 where B is a vector of p fixed effects returned by betta() or betta_random() and L is an m x p matrix with linearly independent rows.

test_submodel 41

Usage

```
test_submodel(
  fitted_betta,
  submodel_formula,
  method = "bootstrap",
  nboot = 1000
)
```

Arguments

fitted_betta

A fitted betta object – i.e., the output of either betta() or betta_random() – containing fixed effect estimates of interest.

submodel_formula

A formula defining which submodel to treat as the null. It is not necessary to include random effects in this formula (they will be ignored if included – the submodel will be fit with the same random effect structure as the full model recordless of input.)

regardless of input.)

method A character variable indicating which method should be used to estimate the

distribution of the test statistic under the null.

nboot Number of bootstrap samples to use if method = "bootstrap". Ignored if method

= "asymptotic".

Value

A list containing

pval The p-value

F_stat The calculated F statistic

boot_F A vector of bootstrapped F statistics if bootstrap has been used. Otherwise

NULL.

Author(s)

David Clausen

References

Willis, A., Bunge, J., and Whitman, T. (2015). Inference for changes in biodiversity. arXiv preprint.

See Also

```
betta;
betta_random;
betta;
F_test
```

42 toy_metadata

Examples

toy_metadata

(Data) Data frame of covariate information about toy_otu_table.

Description

(Data) Data frame of covariate information about toy_otu_table.

Usage

toy_metadata

Format

A data frame with 143 rows and 4 variables:

Years Year of sampling

bloom2 Did the sample correspond to a bloom event?

Period What season was sampled?

Site Where was the sample taken from? ...

toy_otu_table 43

toy_otu_table

(Data) A toy OTU table.

Description

Covariate info available in 'toy_metadata'. A data frame with 448 rows and 143 columns. Rows give the abundance of each taxon; columns give the samples

Usage

```
toy_otu_table
```

Format

An object of class data. frame with 448 rows and 143 columns.

toy_taxonomy

(Data) The taxonomy of the OTUs in 'toy_otu_table'.

Description

(Data) The taxonomy of the OTUs in 'toy_otu_table'.

Usage

toy_taxonomy

Format

An object of class factor of length 448.

true_gini

Calculate the true Gini-Simpson index

Description

Calculate the true Gini-Simpson index

Usage

```
true_gini(input)
```

Arguments

input

A vector of proportions.

Value

The Gini-Simpson index of the population given by input.

44 true_inverse_simpson

Note

This function is intended for population-level data. If you are dealing with a microbial sample, use DivNet instead.

true_hill

Calculate the true Hill numbers

Description

Calculate the true Hill numbers

Usage

```
true_hill(input, q)
```

Arguments

input A vector of proportions.

q The Hill number of interest. q = 0 corresponds to species richness, q = 2 corre-

sponds to inverse Simpson, etc.

Value

The Hill number of the population given by input.

true_inverse_simpson

Calculate the true Inverse Simpson index

Description

Calculate the true Inverse Simpson index

Usage

```
true_inverse_simpson(input)
```

Arguments

input

A vector of proportions.

Value

The inverse-Simpson index of the population given by input.

Note

This function is intended for population-level data. If you are dealing with a microbial sample, use DivNet instead.

true_shannon 45

true_shannon

Calculate the true Shannon index based on proportions

Description

Calculate the true Shannon index based on proportions

Usage

```
true_shannon(input)
```

Arguments

input

A vector of proportions.

Value

The Shannon index of the population given by input.

Note

This function is intended for population-level data. If you are dealing with a microbial sample, use DivNet instead.

true_shannon_e

Calculate the true Shannon's equitability index

Description

Calculate the true Shannon's equitability index

Usage

```
true_shannon_e(input)
```

Arguments

input

A vector of proportions.

Value

The Shannon E's of the population given by input.

Note

This function is intended for population-level data. If you are dealing with a microbial sample, use DivNet instead.

46 wlrm_transformed

true_simpson

Calculate the true Simpson index

Description

Calculate the true Simpson index

Usage

```
true_simpson(input)
```

Arguments

input

A vector of proportions.

Value

The Simpson index of the population given by input.

Note

This function is intended for population-level data. If you are dealing with a microbial sample, use DivNet instead.

wlrm_transformed

The transformed weighted linear regression estimator for species richness estimation

Description

This function implements the transformed version of the species richness estimation procedure outlined in Rocchetti, Bunge and Bohning (2011).

Usage

```
wlrm_transformed(
  input_data,
  cutoff = NA,
  print = NULL,
  plot = NULL,
  answers = NULL
)
```

Arguments

input_data An input type that can be processed by convert() or a phyloseq object

cutoff Maximum frequency count to use

print Deprecated; only for backwards compatibility
plot Deprecated; only for backwards compatibility
answers Deprecated; only for backwards compatibility

wlrm_untransformed 47

Value

An object of class alpha_estimate, or alpha_estimates for phyloseq objects

Note

While robust to many different structures, model is almost always misspecified. The result is usually implausible diversity estimates with artificially low standard errors. Extreme caution is advised.

Author(s)

Amy Willis

References

Rocchetti, I., Bunge, J. and Bohning, D. (2011). Population size estimation based upon ratios of recapture probabilities. *Annals of Applied Statistics*, **5**.

See Also

breakaway; apples; wlrm_untransformed

Examples

```
wlrm_transformed(apples)
wlrm_transformed(apples, plot = FALSE, print = FALSE, answers = TRUE)
```

wlrm_untransformed

The untransformed weighted linear regression estimator for species richness estimation

Description

This function implements the untransformed version of the species richness estimation procedure outlined in Rocchetti, Bunge and Bohning (2011).

Usage

```
wlrm_untransformed(
  input_data,
  cutoff = NA,
  print = NULL,
  plot = NULL,
  answers = NULL
)
```

Arguments

input_data An input type that can be processed by convert() or a phyloseq object

cutoff Maximum frequency count to use

print Deprecated; only for backwards compatibility
plot Deprecated; only for backwards compatibility
answers Deprecated; only for backwards compatibility

48 wlrm_untransformed

Value

An object of class alpha_estimate, or alpha_estimates for phyloseq objects

Note

This estimator is based on the negative binomial model and for that reason generally produces poor fits to microbial data. The result is usually artificially low standard errors. Caution is advised.

Author(s)

Amy Willis

References

Rocchetti, I., Bunge, J. and Bohning, D. (2011). Population size estimation based upon ratios of recapture probabilities. *Annals of Applied Statistics*, **5**.

See Also

breakaway; apples; wlrm_transformed

Examples

wlrm_untransformed(apples)

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