# Package: occumb (via r-universe)

September 13, 2024

```
Title Site Occupancy Modeling for Environmental DNA Metabarcoding Version 1.1.0.9001
```

**Description** Fits multispecies site occupancy models to environmental DNA metabarcoding data collected using spatially-replicated survey design. Model fitting results can be used to evaluate and compare the effectiveness of species detection to find an efficient survey design. Reference: Fukaya et al. (2022) <doi:10.1111/2041-210X.13732>.

```
License GPL (>= 3)
Encoding UTF-8
LazyData true
```

**Roxygen** list(markdown = TRUE)

RoxygenNote 7.3.2

**Suggests** rmarkdown, spelling, testthat (>= 3.0.0)

Config/testthat/edition 3

Imports stats, methods, graphics, checkmate, crayon, knitr

Collate 'classes.R' 'fish.R' 'fish\_raw.R' 'get\_posterior.R' 'gof.R' 'occumbData.R' 'occumb.R' 'plot.R' 'predict.R' 'show.R' 'summary.R' 'utility.R' 'utils.R'

```
URL https://fukayak.github.io/occumb/,
    https://github.com/fukayak/occumb
```

**Depends** jagsUI, R (>= 2.10)

VignetteBuilder knitr

**SystemRequirements** JAGS (http://mcmc-jags.sourceforge.net)

BugReports https://github.com/fukayak/occumb/issues

Language en-US

Repository https://fukayak.r-universe.dev

RemoteUrl https://github.com/fukayak/occumb

RemoteRef HEAD

RemoteSha d969e4e8b1a3ed71fed2233972ec3b20e486769b

# **Contents**

eval_util_L	2
eval_util_R	5
$fish \dots \dots$	9
fish_raw	9
get_posterior	10
gof	12
$list\_cond\_L \ \dots $	13
$list\_cond\_R \ \dots $	14
occumb	15
occumbData	19
plot,occumbFit-method	20
plot,occumbGof-method	21
predict,occumbFit-method	21
summary,occumbData-method	22
summary,occumbFit-method	23
	24
	- 14

eval\_util\_L

Expected utility for local species diversity assessments.

# Description

eval\_util\_L() evaluates the expected utility of a local species diversity assessment by using Monte Carlo integration.

## Usage

Index

```
eval_util_L(
   settings,
   fit = NULL,
   z = NULL,
   theta = NULL,
   phi = NULL,
   N_rep = 1,
   cores = 1L
)
```

## **Arguments**

settings

A data frame that specifies a set of conditions under which utility is evaluated. It must include columns named K and N, which specify the number of replicates per site and the sequencing depth per replicate, respectively. K and N must be numeric vectors greater than 0. When K contains a decimal value, it is discarded and treated as an integer. Additional columns are ignored, but may be included.

fit

An occumbFit object.

Sample values of site occupancy status of species stored in an array with sample Z  $\times$  species  $\times$  site dimensions. theta Sample values of sequence capture probabilities of species stored in a matrix with sample  $\times$  species dimensions or an array with sample  $\times$  species  $\times$  site dimensions. phi Sample values of sequence relative dominance of species stored in a matrix with sample × species dimensions or an array with sample × species × site dimensions. Controls the sample size for the Monte Carlo integration. The integral is eval-N\_rep uated using N\_sample \* N\_rep random samples, where N\_sample is the maximum size of the MCMC sample in the fit argument and the parameter sample in the z, theta, and phi arguments. The number of cores to use for parallelization. cores

#### **Details**

The utility of local species diversity assessment for a given set of sites can be defined as the expected number of detected species per site (Fukaya et al. 2022). eval\_util\_L() evaluates this utility for arbitrary sets of sites that can potentially have different values for site occupancy status of species, z, sequence capture probabilities of species,  $\theta$ , and sequence relative dominance of species,  $\phi$ , for the combination of K and N values specified in the conditions argument. Such evaluations can be used to balance K and N to maximize the utility under a constant budget (possible combinations of K and N under a specified budget and cost values are easily obtained using list\_cond\_L(); see the example below). It is also possible to examine how the utility varies with different K and N values without setting a budget level, which may be useful for determining a satisfactory level of K and N from a purely technical point of view.

The expected utility is defined as the expected value of the conditional utility in the form:

$$U(K, N \mid r, u) = \frac{1}{J} \sum_{j=1}^{J} \sum_{i=1}^{I} \left\{ 1 - \prod_{k=1}^{K} \left( 1 - \frac{u_{ijk} r_{ijk}}{\sum_{m=1}^{I} u_{mjk} r_{mjk}} \right)^{N} \right\}$$

where  $u_{ijk}$  is a latent indicator variable representing the inclusion of the sequence of species i in replicate k at site j, and  $r_{ijk}$  is a latent variable that is proportional to the relative frequency of the sequence of species i, conditional on its presence in replicate k at site j (Fukaya et al. 2022). Expectations are taken with respect to the posterior (or possibly prior) predictive distributions of  $r = \{r_{ijk}\}$  and  $r = \{u_{ijk}\}$ , which are evaluated numerically using Monte Carlo integration. The predictive distributions of r and  $r = u_{ijk}$ , which are evaluated numerically using Monte Carlo integration. The predictive distribution is specified by supplying an occumbFit object containing their posterior (or prior) distribution is specified by supplying a matrix or array of posterior (or prior) samples of parameter values via the  $r = u_{ijk}$ , theta, and phi arguments. Higher approximation accuracy can be obtained by increasing the value of  $r = u_{ijk}$ .

The eval\_util\_L() function can be executed by supplying the fit argument without specifying the z, theta, and phi arguments, by supplying the three z, theta, and phi arguments without the fit argument, or by supplying the fit argument and any or all of the z, theta, and phi arguments. If z, theta, or phi arguments are specified in addition to the fit, the parameter values given in these arguments are used preferentially to evaluate the expected utility. If the sample sizes differ

among parameters, parameters with smaller sample sizes are resampled with replacements to align the sample sizes across parameters.

The expected utility is evaluated assuming homogeneity of replicates, in the sense that  $\theta$  and  $\phi$ , the model parameters associated with the species detection process, are constant across replicates within a site. For this reason, eval\_util\_L() does not accept replicate-specific  $\theta$  and  $\phi$ . If the occumbFit object supplied in the fit argument has a replicate-specific parameter, the parameter samples to be used in the utility evaluation must be provided explicitly via the theta or phi arguments.

The Monte Carlo integration is executed in parallel on multiple CPU cores, where the cores argument controls the degree of parallelization.

#### Value

A data frame with a column named Utility in which the estimates of the expected utility are stored. This is obtained by adding the Utility column to the data frame provided in the settings argument.

#### References

K. Fukaya, N. I. Kondo, S. S. Matsuzaki and T. Kadoya (2022) Multispecies site occupancy modelling and study design for spatially replicated environmental DNA metabarcoding. *Methods in Ecology and Evolution* **13**:183–193. doi:10.1111/2041210X.13732

```
set.seed(1)
# Generate a random dataset (20 species * 2 sites * 2 reps)
I <- 20 # Number of species
J <- 2 # Number of sites
K <- 2 \# Number of replicates
data <- occumbData(</pre>
    y = array(sample.int(I * J * K), dim = c(I, J, K)))
# Fitting a null model
fit <- occumb(data = data)</pre>
## Estimate expected utility
# Arbitrary K and N values
(util1 <- eval_util_L(expand.grid(K = 1:3, N = c(1E3, 1E4, 1E5)),
                       fit))
# K and N values under specified budget and cost
(util2 <- eval_util_L(list_cond_L(budget = 1E5,</pre>
                                    lambda1 = 0.01,
                                    lambda2 = 5000,
                                    fit),
                       fit))
# K values restricted
(util3 <- eval_util_L(list_cond_L(budget = 1E5,</pre>
```

```
lambda1 = 0.01,
                                   lambda2 = 5000,
                                   fit,
                                   K = 1:5),
                      fit))
# theta and phi values supplied
(util4 <- eval_util_L(list_cond_L(budget = 1E5,</pre>
                                   lambda1 = 0.01,
                                   lambda2 = 5000,
                                   fit,
                                   K = 1:5),
                      fit,
                      theta = array(0.5, dim = c(4000, I, J)),
                      phi = array(1, dim = c(4000, I, J)))
# z, theta, and phi values, but no fit object supplied
(util5 <- eval_util_L(list_cond_L(budget = 1E5,</pre>
                                   lambda1 = 0.01,
                                   lambda2 = 5000,
                                   fit,
                                   K = 1:5),
                      fit = NULL,
                      z = array(1, dim = c(4000, I, J)),
                      theta = array(0.5, dim = c(4000, I, J)),
                      phi = array(1, dim = c(4000, I, J)))
```

eval\_util\_R

Expected utility for regional species diversity assessments.

## **Description**

eval\_util\_R() evaluates the expected utility of a regional species diversity assessment using Monte Carlo integration.

## Usage

```
eval_util_R(
   settings,
   fit = NULL,
   psi = NULL,
   theta = NULL,
   phi = NULL,
   N_rep = 1,
   cores = 1L
)
```

#### **Arguments**

settings A data frame that specifies a set of conditions under which utility is evaluated. It must include columns named J, K, and N, which specify the number of sites, number of replicates per site, and sequencing depth per replicate, respectively. J, K, and N must be numeric vectors greater than 0. When J and K contain decimal values, they are discarded and treated as integers. Additional columns are ignored, but may be included. fit An occumbFit object. Sample values of the site occupancy probabilities of species stored in a matrix psi with sample  $\times$  species dimensions or an array with sample  $\times$  species  $\times$  site dimensions. theta Sample values of sequence capture probabilities of species stored in a matrix with sample  $\times$  species dimensions or an array with sample  $\times$  species  $\times$  site dimensions. phi Sample values of sequence relative dominance of species stored in a matrix with sample  $\times$  species dimensions or an array with sample  $\times$  species  $\times$  site dimensions sions. N\_rep Controls the sample size for the Monte Carlo integration. The integral is evaluated using a total of N\_sample \* N\_rep random samples, where N\_sample is

sample in the psi, theta, and phi arguments.

The number of cores to use for parallelization.

# Details

cores

The utility of a regional species diversity assessment can be defined as the number of species expected to be detected in the region of interest (Fukaya et al. 2022). eval\_util\_R() evaluates this utility for the region modeled in the occumbFit object for the combination of J, K, and N values specified in the conditions argument. Such evaluations can be used to balance J, K, and N to maximize the utility under a constant budget (possible combinations of J, K, and N under a specified budget and cost values are easily obtained using list\_cond\_R(); see the example below). It is also possible to examine how the utility varies with different J, K, and N values without setting a budget level, which may be useful in determining the satisfactory levels of J, K, and N from a purely technical point of view.

the maximum size of the MCMC sample in the fit argument and the parameter

The expected utility is defined as the expected value of the conditional utility in the form:

$$U(J, K, N \mid r, u) = \sum_{i=1}^{I} \left\{ 1 - \prod_{j=1}^{J} \prod_{k=1}^{K} \left( 1 - \frac{u_{ijk} r_{ijk}}{\sum_{m=1}^{I} u_{mjk} r_{mjk}} \right)^{N} \right\}$$

where  $u_{ijk}$  is a latent indicator variable representing the inclusion of the sequence of species i in replicate k at site j, and  $r_{ijk}$  is a latent variable that is proportional to the relative frequency of the sequence of species i, conditional on its presence in replicate k at site j (Fukaya et al. 2022). Expectations are taken with respect to the posterior (or possibly prior) predictive distributions of  $r = \{r_{ijk}\}$  and  $r = \{u_{ijk}\}$ , which are evaluated numerically using Monte Carlo integration. The predictive distributions of r and  $r = u_{ijk}$  are evaluated numerically using Monte Carlo integration. The predictive distributions of  $r = u_{ijk}$  and  $u = u_{ijk}$  and  $u = u_{ijk}$  are evaluated numerically using Monte Carlo integration. The predictive distributions of  $r = u_{ijk}$  and  $u = u_{ijk}$  are evaluated numerically using Monte Carlo integration. The predictive distribution is specified by supplying an occumbFit object containing their posterior

samples via the fit argument, or by supplying a matrix or array of posterior (or prior) samples of parameter values via the psi, theta, and phi arguments. Higher approximation accuracy can be obtained by increasing the value of N\_rep.

The eval\_util\_R() function can be executed by supplying the fit argument without specifying the psi, theta, and phi arguments, by supplying the three psi, theta, and phi arguments without the fit argument, or by supplying the fit argument and any or all of the psi, theta, and phi arguments. If the psi, theta, or phi arguments are specified in addition to the fit, the parameter values given in these arguments are preferentially used to evaluate the expected utility. If the sample sizes differed among parameters, parameters with smaller sample sizes are resampled with replacements to align the sample sizes across parameters.

The expected utility is evaluated assuming homogeneity of replicates, in the sense that  $\theta$  and  $\phi$ , the model parameters associated with the species detection process, are constant across replicates within a site. For this reason, eval\_util\_R() does not accept replicate-specific  $\theta$  and  $\phi$ . If the occumbFit object supplied in the fit argument has a replicate-specific parameter, the parameter samples to be used in the utility evaluation must be provided explicitly via the theta or phi arguments.

If the parameters are modeled as a function of site covariates in the fit object, or if the psi, theta, and/or phi arguments have site dimensions, the expected utility is evaluated to account for the site heterogeneity of the parameters. To incorporate site heterogeneity, the parameter values for each J site are determined by selecting site-specific parameter values in the fit, or those supplied in psi, theta, and phi via random sampling with replacement. Thus, expected utility is evaluated by assuming a set of supplied parameter values as a statistical population of site-specific parameters.

The Monte Carlo integration is executed in parallel on multiple CPU cores, where the cores argument controls the degree of parallelization.

### Value

A data frame with a column named Utility in which the estimates of the expected utility are stored. This is obtained by adding the Utility column to the data frame provided in the settings argument.

## References

K. Fukaya, N. I. Kondo, S. S. Matsuzaki and T. Kadoya (2022) Multispecies site occupancy modelling and study design for spatially replicated environmental DNA metabarcoding. *Methods in Ecology and Evolution* **13**:183–193. doi:10.1111/2041210X.13732

```
set.seed(1)

# Generate a random dataset (20 species * 2 sites * 2 reps)
I <- 20 # Number of species
J <- 2 # Number of sites
K <- 2 # Number of replicates
data <- occumbData(
    y = array(sample.int(I * J * K), dim = c(I, J, K)))
# Fitting a null model</pre>
```

```
fit <- occumb(data = data)</pre>
## Estimate expected utility
# Arbitrary J, K, and N values
(util1 \leftarrow eval\_util_R(expand.grid(J = 1:3, K = 1:3, N = c(1E3, 1E4, 1E5)),
# J, K, and N values under specified budget and cost
(util2 <- eval_util_R(list_cond_R(budget = 50000,</pre>
                                    lambda1 = 0.01,
                                    lambda2 = 5000,
                                    lambda3 = 5000),
                       fit))
# K values restricted
(util3 <- eval_util_R(list_cond_R(budget = 50000,</pre>
                                    lambda1 = 0.01,
                                    lambda2 = 5000,
                                    lambda3 = 5000,
                                   K = 1:5),
                       fit))
# J and K values restricted
(util4 <- eval_util_R(list_cond_R(budget = 50000,</pre>
                                    lambda1 = 0.01,
                                    lambda2 = 5000,
                                    lambda3 = 5000,
                                    J = 1:3, K = 1:5),
                       fit))
# theta and phi values supplied
(util5 <- eval_util_R(list_cond_R(budget = 50000,</pre>
                                    lambda1 = 0.01,
                                    lambda2 = 5000,
                                    lambda3 = 5000,
                                    J = 1:3, K = 1:5),
                       fit,
                       theta = array(0.5, dim = c(4000, I, J)),
                       phi = array(1, dim = c(4000, I, J)))
# psi, theta, and phi values, but no fit object supplied
(util6 <- eval_util_R(list_cond_R(budget = 50000,</pre>
                                    lambda1 = 0.01,
                                    lambda2 = 5000,
                                    lambda3 = 5000,
                                    J = 1:3, K = 1:5),
                       fit = NULL,
                       psi = array(0.9, dim = c(4000, I, J)),
                       theta = array(0.9, dim = c(4000, I, J)),
                       phi = array(1, dim = c(4000, I, J)))
```

fish 9

fish

Fish eDNA metabarcoding dataset

#### **Description**

A dataset of fish eDNA metabarcoding collected in the Kasumigaura watershed, Japan.

## Usage

fish

#### **Format**

An occumbData class object containing the sequence read count y, a species covariate mismatch, and a site covariate riverbank. mismatch represents the total number of mismatched bases in the priming region of the forward and reverse primers for each species. riverbank indicates whether the riverbank at each site lacks aquatic and riparian vegetation. Sequence reads were obtained from three replicates (collected from the center of the river and near the left and right riverbanks) from 50 sites across the watershed, of which read counts from six samples were missing. The resulting sequence counts of 50 freshwater fish taxa were recorded.

#### **Source**

K. Fukaya, N. I. Kondo, S. S. Matsuzaki, T. Kadoya (2021) Data from: Multispecies site occupancy modeling and study design for spatially replicated environmental DNA metabarcoding. Dryad Digital Repository. doi:10.5061/dryad.3bk3j9kkm

fish\_raw

Fish eDNA metabarcoding dataset

## **Description**

A dataset of fish eDNA metabarcoding collected in the Kasumigaura watershed, Japan.

#### **Usage**

fish\_raw

#### Format

A list containing an array of sequence read count, y, a vector of the total number of mismatched bases in the priming region of the forward and reverse primers for each species, mismatch, and a factor indicating whether the riverbank at each site lacked aquatic and riparian vegetation, riverbank. Sequence reads were obtained from three replicates (collected from the center of the river and near the left and right riverbanks) from 50 sites across the watershed, of which read counts from six samples were missing. The resulting sequence counts of 50 freshwater fish taxa detected were recorded.

10 get\_posterior

## Source

K. Fukaya, N. I. Kondo, S. S. Matsuzaki, T. Kadoya (2021) Data from: Multispecies site occupancy modeling and study design for spatially replicated environmental DNA metabarcoding. Dryad Digital Repository. doi:10.5061/dryad.3bk3j9kkm

get\_posterior

Extract posterior samples or summary of parameters from a model-fit object.

## Description

get\_post\_samples() extracts posterior samples of the specified parameters from a model-fit object.

get\_post\_summary() extracts posterior summary of the specified parameters from a model-fit object.

## Usage

```
get_post_samples(
   fit,
   parameter = c("z", "pi", "phi", "theta", "psi", "alpha", "beta", "gamma",
        "alpha_shared", "beta_shared", "gamma_shared", "Mu", "sigma", "rho")
)

get_post_summary(
   fit,
   parameter = c("z", "pi", "phi", "theta", "psi", "alpha", "beta", "gamma",
        "alpha_shared", "beta_shared", "gamma_shared", "Mu", "sigma", "rho")
)
```

## Arguments

fit An occumbFit object.

parameter A string of parameter

A string of parameter name. See Details for possible choices and corresponding parameters.

## **Details**

The functions return posterior samples or a summary of one of the following parameters in the model, stored in the model-fit object fit:

- z Site occupancy status of species.
- pi Multinomial probabilities of species sequence read counts.
- phi Sequence relative dominance of species.

theta Sequence capture probabilities of species.

get\_posterior 11

```
psi Site occupancy probabilities of species.
```

alpha Species-specific effects on sequence relative dominance (phi).

beta Species-specific effects on sequence capture probabilities (theta).

gamma Species-specific effects on site occupancy probabilities (psi).

alpha\_shared Effects on sequence relative dominance (phi) common across species.

beta\_shared Effects on sequence capture probabilities (theta) that are common across species.

gamma\_shared Effects on site occupancy probabilities (psi) that are common across species.

Mu Community-level averages of species-specific effects (alpha, beta, gamma).

sigma Standard deviations of species-specific effects (alpha, beta, gamma).

rho Correlation coefficients of the species-specific effects (alpha, beta, gamma).

See the package vignette for details of these parameters.

The parameter may have dimensions corresponding to species, sites, replicates, and effects (covariates) and the dimension and label attributes are added to the output object to inform these dimensions. If the sequence read count data y have species, site, or replicate names appended as the dimnames attribute (see Details in occumbData()), they are copied into the label attribute of the returned object.

#### Value

get\_post\_samples() returns a vector, matrix, or array of posterior samples for a selected parameter

get\_post\_summary() returns a table (matrix) of the posterior summary of the selected parameters. The elements of the posterior summary are the same as those obtained with the jags() function in the jagsUI package: they include the mean, standard deviation, percentiles of posterior samples; the Rhat statistic; the effective sample size, n.eff; overlap0, which checks if 0 falls in the parameter's 95% credible interval; and the proportion of the posterior with the same sign as the mean, f.

The dimension and label attributes of the output object provide information regarding the dimensions of the parameter.

12 gof

```
attributes(post_sample_z)
# Extract posterior summary
(post_summary_z <- get_post_summary(fit, "z"))
# Look dimensions of the parameter
attributes(post_summary_z)</pre>
```

gof

Goodness-of-fit assessment of the fitted model.

## **Description**

gof() calculates omnibus discrepancy measures and their Bayesian p-values for the fitted model using the posterior predictive check approach.

## Usage

```
gof(fit, stats = c("Freeman_Tukey", "deviance"), cores = 1L, plot = TRUE, ...)
```

## **Arguments**

fit	An occumbFit object.
stats	The discrepancy statistics to be applied.
cores	The number of cores to use for parallelization.
plot	Logical, determine if draw scatter plots of the fit statistics.
	Additional arguments passed to the default plot method.

#### **Details**

A discrepancy statistic for the fitted model is obtained using a posterior predictive checking procedure. The following statistics are currently available:

Freeman-Tukey statistics (default) 
$$T_{\text{FT}} = \sum_{i,j,k} \left( \sqrt{y_{ijk}} - \sqrt{E(y_{ijk} \mid \pi_{ijk})} \right)^2$$
  
Deviance statistics  $T_{\text{deviance}} = -2 \sum_{j,k} \log \text{Multinomial}(\boldsymbol{y}_{jk} \mid \boldsymbol{\pi}_{jk})$ 

where i,j, and k are the subscripts of species, site, and replicate, respectively,  $y_{ijk}$  is sequence read count data,  $\pi_{ijk}$  is multinomial cell probabilities of sequence read counts,  $E(y_{ijk} \mid \pi_{ijk})$  is expected value of the sequence read counts conditional on their cell probabilities, and log Multinomial  $(y_{jk} \mid \pi_{jk})$  is the multinomial log-likelihood of the sequence read counts in replicate k of site j conditional on their cell probabilities.

The Bayesian p-value is estimated as the probability that the value of the discrepancy statistics of the replicated dataset is more extreme than that of the observed dataset. An extreme Bayesian p-value may indicate inadequate model fit. See Gelman et al. (2014), Kéry and Royle (2016), and Conn et al. (2018) for further details on the procedures used for posterior predictive checking.

Computations can be run in parallel on multiple CPU cores where the cores argument controls the degree of parallelization.

list\_cond\_L 13

#### Value

```
A list with the following named elements:

stats The discrepancy statistics applied.

p_value Bayesian p-value.

stats_obs Discrepancy statistics for observed data.

stats_rep Discrepancy statistics for repeated data.
```

#### References

P. B. Conn, D. S. Johnson, P. J. Williams, S. R. Melin and M. B. Hooten. (2018) A guide to Bayesian model checking for ecologists. *Ecological Monographs* **88**:526–542. doi:10.1002/ecm.1314

A. Gelman, J. B. Carlin, H. S. Stern D. B. Dunson, A. Vehtari and D. B. Rubin (2013) *Bayesian Data Analysis*. 3rd edition. Chapman and Hall/CRC. http://www.stat.columbia.edu/~gelman/book/

M. Kéry and J. A. Royle (2016) Applied Hierarchical Modeling in Ecology — Analysis of Distribution, Abundance and Species Richness in R and BUGS. Volume 1: Prelude and Static Models. Academic Press. https://www.mbr-pwrc.usgs.gov/pubanalysis/keryroylebook/

## **Examples**

list\_cond\_L

Conditions for local assessment under certain budget and cost values.

### **Description**

list\_cond\_L() constructs a list of possible local species diversity assessment conditions under the specified budget and cost values.

14 list\_cond\_R

## Usage

```
list_cond_L(budget, lambda1, lambda2, fit, K = NULL)
```

## **Arguments**

budget	A numeric specifying budget amount. The currency unit is arbitrary but must be consistent with that of lambda1 and lambda2.
lambda1	A numeric specifying the cost per sequence read for high-throughput sequencing. The currency unit is arbitrary but must be consistent with that of budget and lambda2.
lambda2	A numeric specifying the cost per replicate for library preparation. The currency unit is arbitrary but must be consistent with that of budget and lambda1.
fit	An occumbFit object.
K	An optional vector for manually specifying the number of replicates.

#### **Details**

This function can generate a data frame object to be given to the settings argument of eval\_util\_L(); see Examples of eval\_util\_L(). By default, it outputs a list of all feasible combinations of values for the number of replicates per site K and the sequencing depth per replicate N based on the given budget, cost values, and number of sites (identified by reference to the fit object). The resulting N can be a non-integer because it is calculated simply by assuming that the maximum value can be obtained. To obtain a list for only a subset of the possible K values under a given budget and cost value, the K argument is used to provide a vector of the desired K values.

## Value

A data frame containing columns named budget, lambda1, lambda2, K, and N.

list_cond_R	Conditions for regional assessment under certain budget and cost val-
	ues.

# **Description**

list\_cond\_R() constructs a list of possible regional species diversity assessment conditions under the specified budget and cost values.

### Usage

```
list_cond_R(budget, lambda1, lambda2, lambda3, J = NULL, K = NULL)
```

#### **Arguments**

budget	A numeric specifying budget amount. The currency unit is arbitrary but must be consistent with that of lambda1, lambda2, and lambda3.
lambda1	A numeric specifying the cost per sequence read for high-throughput sequencing. The currency unit is arbitrary but must be consistent with that of budget, lambda2, and lambda3.
lambda2	A numeric specifying the cost per replicate for library preparation. The currency unit is arbitrary but must be consistent with that of budget, lambda1, and lambda3.
lambda3	A numeric specifying the visiting cost per site. The currency unit is arbitrary but must be consistent with that of budget, lambda1, and lambda2.
J	An optional vector for manually specifying the number of sites
K	An optional vector used to specify the number of replicates manually. For computational convenience, the K values must be in ascending order.

#### **Details**

This function can generate a data frame object to be given to the settings argument of eval\_util\_R(); see Examples of eval\_util\_R(). By default, it outputs a list of all feasible combinations of values for the number of sites J, number of replicates per site K, and sequencing depth per replicate N based on the given budget and cost values. The resulting N can be a non-integer because it is calculated simply by assuming that the maximum value can be obtained. If one wants to obtain a list for only a subset of the possible values of J and K under a given budget and cost value, use the J and/or K arguments (in fact, it is recommended that a relatively small number of K values be specified using the K argument because the list of all conditions achievable under moderate budget and cost values can be large, and it is rarely practical to have a vast number of replicates per site). If a given combination of J and K values is not feasible under the specified budget and cost values, the combination will be ignored and excluded from the output.

## Value

A data frame containing columns named budget, lambda1, lambda2, lambda3, J, K, and N.

|--|

## **Description**

occumb() fits the multispecies site-occupancy model for eDNA metabarcoding (Fukaya et al. 2022) and returns a model-fit object containing posterior samples.

## Usage

```
occumb(
  formula_phi = \sim 1,
  formula\_theta = ~1,
  formula_psi = ~1,
  formula_phi_shared = ~1,
  formula_theta_shared = ~1,
  formula_psi_shared = ~1,
  prior_prec = 1e-04,
  prior_ulim = 10000,
  data,
  n.chains = 4,
  n.adapt = NULL,
  n.burnin = 10000,
  n.thin = 10,
 n.iter = 20000,
 parallel = FALSE,
)
```

## **Arguments**

formula\_phi A right-hand side formula describing species-specific effects of sequence rela-

tive dominance  $(\phi)$ .

formula\_theta A right-hand side formula describing species-specific effects of sequence cap-

ture probability  $(\theta)$ .

formula\_psi A right-hand side formula describing species-specific effects of occupancy prob-

ability  $(\psi)$ .

formula\_phi\_shared

A right-hand side formula describing effects of sequence relative dominance ( $\phi$ ) that are common across species. The intercept term is ignored (see Details).

formula\_theta\_shared

A right-hand side formula describing effects of sequence capture probability ( $\theta$ ) that are common across species. The intercept term is ignored (see Details).

formula\_psi\_shared

A right-hand side formula describing effects of occupancy probability  $(\psi)$  that

are common across species. The intercept term is ignored (see Details).

prior\_prec Precision of normal prior distribution for the community-level average of species-

specific parameters and effects common across species.

prior\_ulim Upper limit of uniform prior distribution for the standard deviation of species-

specific parameters.

data A dataset supplied as an occumbData class object.

n. chains Number of Markov chains to run.

n.adapt Number of iterations to run in the JAGS adaptive phase.

n.burnin Number of iterations at the beginning of the chain to discard.

n. thin Thinning rate. Must be a positive integer.n. iter Total number of iterations per chain (including burn-in).

parallel If TRUE, run MCMC chains in parallel on multiple CPU cores.

... Additional arguments passed to jags() function.

#### **Details**

occumb() allows the fitting of a range of multispecies site occupancy models, including covariates at different levels of the data generation process. The most general form of the model can be written as follows (the notation follows that of the original article; see References).

Sequence read counts:

$$(y_{1jk},...,y_{Ijk}) \sim \text{Multinomial}((\pi_{1jk},...,\pi_{Ijk}),N_{jk}),$$
 
$$\pi_{ijk} = \frac{u_{ijk}r_{ijk}}{\sum_{m}u_{mjk}r_{mjk}},$$

Relative frequency of species sequences:

$$r_{ijk} \sim \text{Gamma}(\phi_{ijk}, 1),$$

Capture of species sequences:

$$u_{ijk} \sim \text{Bernoulli}(z_{ij}\theta_{ijk}),$$

Site occupancy of species:

$$z_{ij} \sim \text{Bernoulli}(\psi_{ij}),$$

where the variations of  $\phi$ ,  $\theta$ , and  $\psi$  are modeled by specifying model formulas in formula\_phi, formula\_theta, formula\_psi, formula\_phi\_shared, formula\_theta\_shared, and formula\_psi\_shared.

Each parameter may have species-specific effects and effects that are common across species, where the former is specified by formula\_phi, formula\_theta, and formula\_psi, whereas formula\_phi\_shared, formula\_theta\_shared, and formula\_psi\_shared specify the latter. As species-specific intercepts are specified by default, the intercept terms in formula\_phi\_shared, formula\_theta\_shared, and formula\_psi\_shared are always ignored. Covariate terms must be found in the names of the list elements stored in the spec\_cov, site\_cov, or repl\_cov slots in the dataset object provided with the data argument. Covariates are modeled using the log link function for  $\phi$  and logit link function for  $\theta$  and  $\psi$ .

The two arguments, prior\_prec and prior\_ulim, control the prior distribution of parameters. For the community-level average of species-specific effects and effects common across species, a normal prior distribution with a mean of 0 and precision (i.e., the inverse of the variance) prior\_prec is specified. For the standard deviation of species-specific effects, a uniform prior distribution with a lower limit of zero and an upper limit of prior\_ulim is specified. For the correlation coefficient of species-specific effects, a uniform prior distribution in the range of -1 to 1 is specified by default.

See the package vignette for details on the model specifications in occumb().

The data argument requires a dataset object to be generated using ocumbData(); see the document of occumbData().

The model is fit using the jags() function of the jagsUI package, where Markov chain Monte Carlo methods are used to obtain posterior samples of the parameters and latent variables. Arguments n.chains, n.adapt, n.burnin, n.thin, n.iter, and parallel are passed on to arguments of the same name in the jags() function. See the document of jagsUI's jags() function for details.

#### Value

An S4 object of the occumbFit class containing the results of the model fitting and the supplied dataset.

#### References

K. Fukaya, N. I. Kondo, S. S. Matsuzaki and T. Kadoya (2022) Multispecies site occupancy modelling and study design for spatially replicated environmental DNA metabarcoding. *Methods in Ecology and Evolution* **13**:183–193. doi:10.1111/2041210X.13732

```
# Generate the smallest random dataset (2 species * 2 sites * 2 reps)
I <- 2 # Number of species
J <- 2 # Number of sites
K <- 2 # Number of replicates
data <- occumbData(</pre>
    y = array(sample.int(I * J * K), dim = c(I, J, K)),
    spec_cov = list(cov1 = rnorm(I)),
    site_cov = list(cov2 = rnorm(J),
                    cov3 = factor(1:J)),
    repl_cov = list(cov4 = matrix(rnorm(J * K), J, K)))
# Fitting a null model (includes only species-specific intercepts)
res0 <- occumb(data = data)</pre>
# Add species-specific effects of site covariates in occupancy probabilities
res1 <- occumb(formula_psi = ~ cov2, data = data) # Continuous covariate
res2 <- occumb(formula_psi = ~ cov3, data = data)
                                                         # Categorical covariate
res3 <- occumb(formula_psi = ~ cov2 * cov3, data = data) # Interaction
# Add species covariate in the three parameters
# Note that species covariates are modeled as common effects
res4 <- occumb(formula_phi_shared = ~ cov1, data = data) # phi
res5 <- occumb(formula_theta_shared = ~ cov1, data = data) # theta
res6 <- occumb(formula_psi_shared = ~ cov1, data = data) # psi
# Add replicate covariates
# Note that replicate covariates can only be specified for theta and phi
res7 <- occumb(formula_phi = ~ cov4, data = data) # phi
res8 <- occumb(formula_theta = ~ cov4, data = data) # theta
# Specify the prior distribution and MCMC settings explicitly
res9 <- occumb(data = data, prior_prec = 1E-2, prior_ulim = 1E2,
               n.chains = 1, n.burnin = 1000, n.thin = 1, n.iter = 2000)
res10 <- occumb(data = data, parallel = TRUE, n.cores = 2) # Run MCMC in parallel
```

occumbData 19

occumbData	Constructor for occumbData data class.	

## **Description**

occumbData() creates a data list compatible with the model fitting function occumb().

## Usage

```
occumbData(y, spec_cov = NULL, site_cov = NULL, repl_cov = NULL)
```

## **Arguments**

у	A 3-D array of sequence read counts (integer values) that may have a dimnames attribute. The dimensions are ordered by species, site, and replicate. The data for missing replicates are represented by zero vectors. NAs are not allowed.
spec_cov	A named list of species covariates. Each covariate can be a vector of continuous (numeric or integer) or discrete (logical, factor, or character) variables whose length is dim(y)[1] (i.e., the number of species). NAs are not allowed.
site_cov	A named list of site covariates. Each covariate can be a vector of continuous (numeric or integer) or discrete (logical, factor, or character) variables whose length is dim(y)[1] (i.e., the number of sites). NAs are not allowed.
repl_cov	A named list of replicate covariates. Each covariate can be a matrix of continuous (numeric or integer) or discrete (logical or character) variables with dimensions equal to dim(y)[2:3] (i.e., number of sites × number of replicates). NAs are not allowed.

## **Details**

The element (i.e., covariate) names for spec\_cov, site\_cov, and repl\_cov must all be unique. If y has a dimnames attribute, it is retained in the resulting occumbData object, and can be referenced in subsequent analyses.

#### Value

An S4 object of the occumbData class.

```
# Generate the smallest random dataset (2 species * 2 sites * 2 reps)
I <- 2 # Number of species
J <- 2 # Number of sites
K <- 2 # Number of replicates
data <- occumbData(
    y = array(sample.int(I * J * K), dim = c(I, J, K)),
    spec_cov = list(cov1 = rnorm(I)),
    site_cov = list(cov2 = rnorm(J), cov3 = factor(1:J)),</pre>
```

```
repl_cov = list(cov4 = matrix(rnorm(J * K), J, K))
)
# A case for named y (with species and site names)
y_named <- array(sample.int(I * J * K), dim = c(I, J, K))
dimnames(y_named) <- list(c("common species", "uncommon species"),</pre>
                           c("good site", "bad site"), NULL)
data_named <- occumbData(</pre>
    y = y_named,
    spec_cov = list(cov1 = rnorm(I)),
    site_cov = list(cov2 = rnorm(J), cov3 = factor(1:J)),
    repl_cov = list(cov4 = matrix(rnorm(J * K), J, K))
)
# A real data example
data(fish_raw)
fish <- occumbData(</pre>
    y = fish_raw$y,
    spec_cov = list(mismatch = fish_raw$mismatch),
    site_cov = list(riverbank = fish_raw$riverbank)
)
# Get an overview of the datasets
summary(data)
summary(data_named)
summary(fish)
```

plot,occumbFit-method Plot method for occumbFit class.

## Description

Applies jagsUI's plot method to an occumbFit object to draw trace plots and density plots of MCMC samples of model parameters.

## Usage

```
## S4 method for signature 'occumbFit'
plot(x, y = NULL, ...)
```

## **Arguments**

x An occumbFit object.

y NULI

... Additional arguments passed to the plot method for jagsUI object.

## Value

Returns NULL invisibly.

plot,occumbGof-method

plot, occumbGof-method Plot method for occumbGof class.

## **Description**

Draws a scatter plot of fit statistics.

## Usage

```
## S4 method for signature 'occumbGof'
plot(x, y = NULL, ...)
```

## **Arguments**

```
x An occumbGof object.
```

y NULL

... Additional arguments passed to the default plot method.

## Value

Returns NULL invisibly.

```
predict,occumbFit-method
```

 $Predict\ method\ for\ occumb Fit\ class.$ 

# Description

Obtain predictions of parameters related to species occupancy and detection from an occumbFit model object.

## Usage

```
## S4 method for signature 'occumbFit'
predict(
  object,
  newdata = NULL,
  parameter = c("phi", "theta", "psi"),
  scale = c("response", "link"),
  type = c("quantiles", "mean", "samples")
)
```

## Arguments

object An occumbFit object.

newdata An optional occumbData object with covariates to be used for prediction. If

omitted, the fitted covariates are used.

parameter The parameter to be predicted.

scale The scale on which the prediction is made. type = "response" returns the pre-

diction on the original scale of the parameter. type = "link" returns the predic-

tion on the link scale of the parameter.

type The type of prediction. type = "quantiles" returns 50% quantile as the pos-

terior median of the prediction in addition to 2.5 and 97.5% quantiles as the lower and upper limits of the 95% credible interval of the prediction. type = "mean" returns the posterior mean of the prediction. type = "samples" returns

the posterior samples of the prediction.

#### **Details**

Applying predict() to an occumbFit object generates predictions for the specified parameter (phi, theta, or psi) based on the estimated effects and the given covariates. It is important to recognize that the predictions are specific to the individual species being modeled since they depend on the estimated species-specific effects (i.e., alpha, beta, and gamma; see the package vignette for details). When providing newdata, it must thus be assumed that the set of species contained in newdata is the same as that of the data being fitted.

### Value

Predictions are obtained as a matrix or array that can have dimensions corresponding to statistics (or samples), species, sites, and replicates. The dimension and label attributes are added to the output object to inform these dimensions. If the sequence read count data y has species, site, or replicate names appended as the dimnames attribute (see Details in occumbData()), they will be copied into the label attribute of the returned object.

summary, occumbData-method

Summary method for occumbData class.

#### **Description**

Summarizes dataset stored in an occumbData object.

#### Usage

```
## S4 method for signature 'occumbData'
summary(object)
```

## **Arguments**

object An occumbData object.

# Value

Returns NULL invisibly.

```
summary,occumbFit-method
```

Summary method for occumbFit class.

# Description

Summarizes model fitting result stored in an occumbFit object.

# Usage

```
## S4 method for signature 'occumbFit'
summary(object)
```

# Arguments

object

An occumbFit object.

# Value

Returns NULL invisibly.

# **Index**

```
* datasets
    fish, 9
    fish\_raw, 9
eval_util_L, 2
eval_util_R, 5
fish, 9
fish_raw,9
get_post_samples (get_posterior), 10
get_post_summary (get_posterior), 10
get_posterior, 10
gof, 12
jags, 11, 17
list_cond_L, 13
list\_cond\_R, \\ 14
occumb, 15, 19
occumbData, 11, 16, 17, 19, 22
\verb"plot,occumbFit-method," 20"
plot,occumbGof-method, 21
\verb|predict,occumbFit-method,21|
summary, occumbData-method, 22
summary,occumbFit-method, 23
```