# Package 'miaSim'

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Title Microbiome Data Simulation

**Description** Microbiome time series simulation with generalized Lotka-Volterra model, Self-Organized Instability (SOI), and other models. Hubbell's Neutral model is used to determine the abundance matrix. The resulting abundance matrix is applied to (Tree)SummarizedExperiment objects.

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2 .applyInterType

Author Yagmur Simsek [cre, aut],

Karoline Faust [aut],
Yu Gao [aut],
Emma Gheysen [aut],
Daniel Rios Garza [aut],
Tuomas Borman [aut] (<a href="https://orcid.org/0000-0002-8563-8884">https://orcid.org/0000-0002-8563-8884</a>),
Leo Lahti [aut] (<a href="https://orcid.org/0000-0001-5537-637X">https://orcid.org/0000-0001-5537-637X</a>)

Maintainer Yagmur Simsek < yagmur .simsek .98@gmail .com>

# **Contents**

|       | .applyInterType  | 2  |
|-------|--|----|
|       | .estimateAFromSimulations  | 3  |
|       | .eventTimes  | 4  |
|       | .getInteractions   |    |
|       | .isPosInt  | 5  |
|       | rdirichlet   | 6  |
|       | .replaceByZero   | 6  |
|       | .simulationTimes   | 7  |
|       | powerlawA  | 7  |
|       | randomA  | 8  |
|       | randomE  | 11 |
|       | simulateConsumerResource   | 13 |
|       | simulateGLV  | 17 |
|       | simulateHubbell  | 20 |
|       | simulateHubbellRates   |    |
|       | simulateRicker   | 23 |
|       | simulateSOI  |    |
|       | simulateStochasticLogistic   | 26 |
|       |  |    |
| Index |  | 30 |
|       |  |    |
|       |  |    |
|       |  |    |
| .app  | yInterType Generate pairs of interactions according to interaction types |    |

# Description

A helper function to be used in combination with .getInteractions()

# Usage

```
.applyInterType(I, pair, interType)
```

.estimateAFromSimulations

#### Arguments

I Matrix: defining the interaction between each pair of species

pair Numeric: a vector with a length of 2, indicating the 2 focusing species in the

process of applying the interaction types

interType Character: one of 'mutualism', 'commensalism', 'parasitism', 'amensalism', or

'competition'. Defining the interaction type

#### Value

A matrix of interaction types with one pair changed

.estimateAFromSimulations

Get the interspecies interaction matrix A using leave-one-out method

3

#### **Description**

generate matrix A from the comparisons between simulations with one absent species and a simulation with complete species (leave-one-out)

## Usage

```
.estimateAFromSimulations(
   simulations,
   simulations2,
   n_instances = 1,
   t_end = NULL,
   scale_off_diagonal = 0.1,
   diagonal = -0.5,
   connectance = 0.2
)
```

## **Arguments**

simulations A list of simulation(s) with complete species

simulations2 A list of simulation(s), each with one absent species

n\_instances Integer: number of instances to generate (default: n\_instances = 1)

t\_end Numeric: end time of the simulation. If not identical with t\_end in params\_list,

then it will overwrite t\_end in each simulation (default: t\_end = 1000)

scale\_off\_diagonal

Numeric: scale of the off-diagonal elements compared to the diagonal. Same to the parameter in function randomA. (default: scale\_off\_diagonal = 0.1)

diagonal Values definir

Values defining the strength of self-interactions. Input can be a number (will be applied to all species) or a vector of length n\_species. Positive self-interaction values lead to exponential growth. Same to the parameter in function randomA.

(default: diagonal = -0.5)

4 .eventTimes

connectance

Numeric frequency of inter-species interactions. i.e. proportion of non-zero off-diagonal terms. Should be in the interval  $0 \le \text{connectance} \le 1$ . Same to the parameter in function randomA. (default: connectance = 0.2)

#### Value

a matrix A with dimensions (n\_species x n\_species) where n\_species equals to the number of elements in simulations2

.eventTimes

generate a vector of times when events is happening

# Description

generate a vector of times when events is happening

#### Usage

```
.eventTimes(t_events = NULL, t_duration = NULL, t_end = 1000, ...)
```

# **Arguments**

```
t_events, t_duration
```

Numeric: vector of starting time and duration of the events

t\_end

Numeric: end time of the simulation

. . . : additional parameters to pass to simulationTimes, including t\_start, t\_step, and

t store.

## Value

A vector of time points in the simulation

```
tEvent <- .eventTimes(
    t_events = c(10, 50, 100),
    t_duration = c(1, 2, 3),
    t_end = 100,
    t_store = 100,
    t_step = 1
)</pre>
```

.getInteractions 5

|  | and their |
|--|-----------|
|--|-----------|

# **Description**

Generate interactions according to five types of interactions and their weights

# Usage

```
.getInteractions(n_species, weights, connectance)
```

# **Arguments**

n\_species Integer: defining the dimension of matrix of interaction

weights Numeric: defining the weights of mutualism, commensalism, parasitism, amen-

salism, and competition in all interspecies interactions.

connectance Numeric: defining the density of the interaction network. Ranging from 0 to 1

#### Value

A matrix of interactions with all interactions changed according to the weights and connectance.

. isPosInt check whether a number is a positive integer

# Description

check whether a number is a positive integer

#### Usage

```
.isPosInt(x, tol = .Machine$double.eps^0.5)
```

# **Arguments**

x Numeric number to test

tol Numeric tolerance of detection

#### Value

A logical value: whether the number is a positive integer.

6 .replaceByZero

.rdirichlet

Generate dirichlet random deviates

# **Description**

Generate dirichlet random deviates

# Usage

```
.rdirichlet(n, alpha)
```

# **Arguments**

Number of random vectors to generate. n

Vector containing shape parameters. alpha

#### Value

a vector containing the Dirichlet density

# **Examples**

```
dirichletExample <- .rdirichlet(1, c(1, 2, 3))</pre>
```

.replaceByZero

Replace one element with zero in a list.

#### **Description**

If the list contains m elements, then lengths of each element must be m, too. This function is intended to generate a list of x0 (the initial community) with one missing species, to prepare the parameter simulations\_compare in estimateAFromSimulations.

# Usage

```
.replaceByZero(input_list)
```

# **Arguments**

input\_list

A list containing m elements, and lengths of each element must be m, too.

#### Value

A list of same dimension as input\_list, but with 0 at specific positions in the elements of the list.

.simulationTimes 7

| .simulationTimes | Generate simulation times and the indices of time points to return in simulation functions. |
|------------------|---|
|------------------|---|

# **Description**

Generate simulation times and the indices of time points to return in simulation functions.

#### Usage

```
.simulationTimes(t_start = 0, t_end = 1000, t_step = 0.1, t_store = 1000)
```

### **Arguments**

| t_start | Numeric scalar indicating the initial time of the simulation. (default: t_start = 0)                    |
|---------|---|
| t_end   | Numeric scalar indicating the final time of the simulation (default: $t_{end} = 1000$ )                 |
| t_step  | Numeric scalar indicating the interval between simulation steps (default: $t_step = 0.1$ )              |
| t_store | Integer scalar indicating the number of evenly distributed time points to keep (default: t_store = 100) |

#### Value

lists containing simulation times (t\_sys) and the indices to keep.

#### **Examples**

```
Time <- .simulationTimes(
    t_start = 0, t_end = 100, t_step = 0.5,
    t_store = 100
)
DefaultTime <- .simulationTimes(t_end = 1000)</pre>
```

powerlawA

Interaction matrix with Power-Law network adjacency matrix

# Description

N is the an Interspecific Interaction matrix with values drawn from a normal distribution H the interaction strength heterogeneity drawn from a power-law distribution with the parameter alpha, and G the adjacency matrix of with out-degree that reflects the heterogeneity of the powerlaw. A scaling factor s may be used to constrain the values of the interaction matrix to be within a desired range. Diagonal elements of A are defined by the parameter d.

8 randomA

# Usage

```
powerlawA(n_species, alpha = 3, stdev = 1, s = 0.1, d = -1, symmetric = FALSE)
```

# Arguments

| n_species | integer number of species   |
|-----------|---|
| alpha     | numeric power-law distribution parameter. Should be > 1. (default: alpha = 3.0) Larger values will give lower interaction strength heterogeneity, whereas values closer to 1 give strong heterogeneity in interaction strengths between the species. In other words, values of alpha close to 1 will give Strongly Interacting Species (SIS). |
| stdev     | numeric standard deviation parameter of the normal distribution with mean 0 from which the elements of the nominal interspecific interaction matrix $N$ are drawn. (default: $stdev = 1$ )  |
| S         | numeric scaling parameter with which the final global interaction matrix A is multiplied. (default: $s = 0.1$ )   |
| d         | numeric diagonal values, indicating self-interactions (use negative values for stability). (default: $s=1.0$ )  |
| symmetric | $logical\ scalar\ returning\ a\ symmetric\ interaction\ matrix\ (default:\ symmetric=FALSE)$  |

#### Value

The interaction matrix A with dimensions (n\_species x n\_species)

# References

Gibson TE, Bashan A, Cao HT, Weiss ST, Liu YY (2016) On the Origins and Control of Community Types in the Human Microbiome. PLOS Computational Biology 12(2): e1004688. https://doi.org/10.1371/journal.pcbi.1004

# **Examples**

```
# Low interaction heterogeneity
A_low <- powerlawA(n_species = 10, alpha = 3)
# Strong interaction heterogeneity
A_strong <- powerlawA(n_species = 10, alpha = 1.01)</pre>
```

randomA Generate random interaction matrix for GLV model

# Description

Generates a random interaction matrix for Generalized Lotka-Volterra (GLV) model.

randomA 9

# Usage

```
randomA(
    n_species,
    names_species = NULL,
    diagonal = -0.5,
    connectance = 0.2,
    scale_off_diagonal = 0.1,
    mutualism = 1,
    commensalism = 1,
    parasitism = 1,
    amensalism = 1,
    competition = 1,
    interactions = NULL,
    symmetric = FALSE,
    list_A = NULL
)
```

# Arguments

| n_species       | Integer: number of species   |
|-----------------|--|
| names_species   | Character: names of species. If NULL, paste0("sp", seq_len(n_species)) is used. (default: names_species = NULL)  |
| diagonal        | Values defining the strength of self-interactions. Input can be a number (will be applied to all species) or a vector of length n_species. Positive self-interaction values lead to exponential growth. (default: diagonal = $-0.5$ )  |
| connectance     | Numeric frequency of inter-species interactions. i.e. proportion of non-zero off-diagonal terms. Should be in the interval $0 \le connectance \le 1$ . (default: connectance = $0.2$ )   |
| scale_off_diago | onal   |
|                 | Numeric: scale of the off-diagonal elements compared to the diagonal. (default: $scale_off_diagonal = 0.1$ )   |
| mutualism       | Numeric: relative proportion of interactions terms consistent with mutualism (positive <-> positive) (default: mutualism = 1)  |
| commensalism    | Numeric: relative proportion of interactions terms consistent with commensalism (positive <-> neutral) (default: $commensalism = 1$ )  |
| parasitism      | Numeric: relative proportion of interactions terms consistent with parasitism (positive $<->$ negative) (default: parasitism = 1)  |
| amensalism      | Numeric: relative proportion of interactions terms consistent with amensalism (neutral $<->$ negative) (default: amensalism = 1)   |
| competition     | Numeric: relative proportion of interactions terms consistent with competition (negative $\leftarrow$ negative) (default: competition = 1)   |
| interactions    | Numeric: values of the n_species^2 pairwise interaction strengths. Diagonal terms will be replaced by the 'diagonal' parameter If NULL, interactions are drawn from runif(n_species^2, min=0, max=abs(diagonal)). Negative values are first converted to positive then the signs are defined by the relative |

10 randomA

weights of the biological interactions (i.e. mutualism, commensalism, parasitism, amensalism, competition) (default: interactions = NULL)

Logical: whether the strength of mutualistic and competitive interactions are symmetric. This is implemented by overwrite a half of the matrix, so the proportions of interactions might deviate from expectations. (default: symmetric=FALSE)

list\_A List: a list of matrices generated by randomA. Used to support different groups of interactions. If NULL (by default), no group is considered. Otherwise the given list of matrices will overwrite values around the diagonal. (default: list\_A

= NULL)

#### Value

symmetric

randomA returns a matrix A with dimensions (n\_species x n\_species)

```
dense_A <- randomA(</pre>
    n_{species} = 10,
    scale_off_diagonal = 1,
    diagonal = -1.0,
    connectance = 0.9
)
sparse_A <- randomA(</pre>
    n_{species} = 10,
    diagonal = -1.0,
    connectance = 0.09
)
user_interactions <- rbeta(n = 10^2, .5, .5)
user_A <- randomA(n_species = 10, interactions = user_interactions)</pre>
competitive_A <- randomA(</pre>
    n_{species} = 10,
    mutualism = 0,
    commensalism = 0,
    parasitism = 0,
    amensalism = 0,
    competition = 1,
    connectance = 1,
    scale_off_diagonal = 1
)
parasitism_A <- randomA(</pre>
    n_{species} = 10,
    mutualism = 0,
    commensalism = 0,
    parasitism = 1,
    amensalism = 0,
    competition = 0,
    connectance = 1,
```

randomE 11

```
scale_off_diagonal = 1,
    symmetric = TRUE
)

list_A <- list(dense_A, sparse_A, competitive_A, parasitism_A)
groupA <- randomA(n_species = 40, list_A = list_A)</pre>
```

randomE

Generate random efficiency matrix

# **Description**

Generate random efficiency matrix for consumer resource model from Dirichlet distribution, where positive efficiencies indicate the consumption of resources, whilst negatives indicate that the species would produce the resource.

## Usage

```
randomE(
   n_species,
   n_resources,
   names_species = NULL,
   names_resources = NULL,
   mean_consumption = n_resources/4,
   mean_production = n_resources/6,
   maintenance = 0.5,
   trophic_levels = NULL,
   trophic_preferences = NULL,
   exact = FALSE
)
```

#### Arguments

Numeric: mean number of resources produced by each species drawn from a poisson distribution (default: mean\_production = n\_resources/6)

12 randomE

maintenance

Numeric: proportion of resources that cannot be converted into products between 0~1 the proportion of resources used to maintain the living of microorganisms. 0 means all the resources will be used for the reproduction of microorganisms, and 1 means all the resources would be used to maintain the living of organisms and no resources would be left for their growth(reproduction). (default: maintenance = 0.5)

trophic\_levels Integer: number of species in microbial trophic levels. If NULL, by default, microbial trophic levels would not be considered. (default: trophic\_levels = NULL)

trophic\_preferences

List: preferred resources and productions of each trophic level. Positive values indicate the consumption of resources, whilst negatives indicate that the species would produce the resource.

exact

Logical: whether to set the number of consumption/production to be exact as mean\_consumption/mean\_production or to set them using a Poisson distribution. (default: exact = FALSE) If length(trophic\_preferences) is smaller than length(trophic\_levels), then NULL values would be appended to lower trophic levels. If NULL, by default, the consumption preference will be defined randomly. (default: trophic\_preferences = NULL)

#### Value

randomE returns a matrix E with dimensions (n\_species x n\_resources), and each row represents a species.

```
# example with minimum parameters
ExampleEfficiencyMatrix <- randomE(n_species = 5, n_resources = 12)</pre>
# examples with specific parameters
ExampleEfficiencyMatrix <- randomE(</pre>
    n_species = 3, n_resources = 6,
   names_species = letters[1:3],
    names_resources = paste0("res", LETTERS[1:6]),
    mean_consumption = 3, mean_production = 1
)
ExampleEfficiencyMatrix <- randomE(</pre>
   n_species = 3, n_resources = 6,
    maintenance = 0.4
)
ExampleEfficiencyMatrix <- randomE(</pre>
    n_species = 3, n_resources = 6,
    mean_consumption = 3, mean_production = 1, maintenance = 0.4
# examples with microbial trophic levels
ExampleEfficiencyMatrix <- randomE(</pre>
    n_species = 10, n_resources = 15,
    trophic_levels = c(6, 3, 1),
```

simulateConsumerResource 13

simulateConsumerResource

Consumer-resource model simulation

### **Description**

Simulates time series with the consumer-resource model.

#### Usage

```
simulateConsumerResource(
 n_species,
 n_resources,
 names_species = NULL,
  names_resources = NULL,
 E = NULL
 x0 = NULL,
  resources = NULL,
  resources_dilution = NULL,
  growth_rates = NULL,
 monod_constant = NULL,
  sigma_drift = 0.001,
  sigma_epoch = 0.1,
  sigma_external = 0.3,
  sigma_migration = 0.01,
  epoch_p = 0.001,
  t_external_events = NULL,
  t_external_durations = NULL,
  stochastic = FALSE,
 migration_p = 0.01,
 metacommunity_probability = NULL,
```

```
error_variance = 0,
norm = FALSE,
t_end = 1000,
trophic_priority = NULL,
inflow_rate = 0,
outflow_rate = 0,
volume = 1000,
...
)
```

#### **Arguments**

n\_species Integer: number of species
n\_resources Integer: number of resources
names\_species Character: names of species. If NULL, paste0("sp", seq\_len(n\_species))

is used. (default: names\_species = NULL)

names\_resources

Character: names of resources. If NULL, paste0("res", seq\_len(n\_resources))

is used.

E matrix: matrix of efficiency. A matrix defining the efficiency of resource-to-

biomass conversion (positive values) and the relative conversion of metabolic by-products (negative values). If NULL, randomE( $n_species, n_resources$ )

is used. (default: E = NULL)

x0 Numeric: initial abundances of simulated species. If NULL, runif(n = n\_species,

min = 0.1, max = 10) is used. (default: x0 = NULL)

resources Numeric: initial concentrations of resources. If NULL, runif(n = n\_resources,

min = 1, max = 100) is used. (default: resources = NULL)

resources\_dilution

Numeric: concentrations of resources in the continuous inflow (applicable when  $inflow_rate > 0$ ). If NULL, resources is used. (default: resources\_dilution

= NULL)

growth\_rates Numeric: vector of maximum growth rates(mu) of species. If NULL, rep(1,

n\_species) is used. (default: growth\_rates = NULL)

monod\_constant matrix: the constant of additive monod growth of n species consuming n resources.

If NULL, matrix(rgamma(n = n\_species\*n\_resources, shape = 50\*max(resources),

rate = 1), nrow = n\_species) is used. (default: monod\_constant = NULL)

sigma\_drift Numeric: standard deviation of a normally distributed noise applied in each time

step (t\_step) (default: sigma\_drift = 0.001)

periods of the community composition with frequency defined by the epoch\_p

parameter (default: sigma\_epoch = 0.1)

sigma\_external Numeric: standard deviation of a normally distributed noise applied to user-

defined external events/disturbances (default: sigma\_external = 0.3)

sigma\_migration

Numeric: standard deviation of a normally distributed variable that defines the intensity of migration at each time step  $(t\_step)$  (default: sigma\_migration =

0.01)

simulateConsumerResource 15

epoch\_p Numeric: the probability/frequency of random periodic changes introduced to the community composition (default:  $epoch_p = 0.001$ )

#### t\_external\_events

Numeric: the starting time points of defined external events that introduce random changes to the community composition (default: t\_external\_events = NULL)

#### t\_external\_durations

Numeric: respective duration of the external events that are defined in the 't\_external\_events' (times) and sigma\_external (std). (default: t\_external\_durations = NULL)

stochastic Logical: whether to introduce noise in the simulation. If False, sigma\_drift, sigma epoch, and sigma external are ignored. (default: stochastic = FALSE)

Numeric: the probability/frequency of migration from a metacommunity. (demigration\_p fault: migration\_p = 0.01)

#### metacommunity\_probability

Numeric: Normalized probability distribution of the likelihood that species from the metacommunity can enter the community during the simulation. If NULL, rdirichlet(1, alpha = rep(1,n\_species)) is used. (default: metacommunity\_probability = NULL)

error\_variance Numeric: the variance of measurement error. By default it equals to 0, indicating that the result won't contain any measurement error. This value should be nonnegative. (default: error\_variance = 0)

norm

Logical: whether the time series should be returned with the abundances as proportions (norm = TRUE) or the raw counts (default: norm = FALSE) (default: norm = FALSE)

t\_end

Numeric: the end time of the simulationTimes, defining the modeled time length of the community. (default: t\_end = 1000)

# trophic\_priority

Matrix: a matrix defining the orders of resources to be consumed by each species. If NULL, by default, this feature won't be turned on, and species will consume all resources simultaneously to grow. The dimension should be identical to matrix E. (default: trophic\_priority = NULL)

#### inflow\_rate, outflow\_rate

Numeric: the inflow and outflow rate of a culture process. By default, inflow\_rate and outflow\_rate are 0, indicating a batch culture process. By setting them equally larger than 0, we can simulate a continuous culture(e.g. chemostat).

volume

Numeric: the volume of the continuous cultivation. This parameter is important for simulations where inflow\_rate or outflow\_rate are not 0. (default: volume = 1000)

additional parameters, see utils to know more.

#### Value

an TreeSummarizedExperiment class object

```
n_species <- 2
n_resources <- 4
tse <- simulateConsumerResource(</pre>
    n_species = n_species,
    n_resources = n_resources
# example with user-defined values (names_species, names_resources, E, x0,
# resources, growth_rates, error_variance, t_end, t_step)
ExampleE <- randomE(</pre>
    n_species = n_species, n_resources = n_resources,
    mean_consumption = 3, mean_production = 1, maintenance = 0.4
)
ExampleResources <- rep(100, n_resources)</pre>
tse1 <- simulateConsumerResource(</pre>
    n_species = n_species,
    n_resources = n_resources, names_species = letters[seq_len(n_species)],
    names_resources = paste0("res", LETTERS[seq_len(n_resources)]), E = ExampleE,
    x0 = rep(0.001, n\_species), resources = ExampleResources,
    growth_rates = runif(n_species),
    error_variance = 0.01,
    t_{end} = 5000,
    t_step = 1
)
# example with trophic levels
n_species <- 10
n_resources <- 15
ExampleEfficiencyMatrix <- randomE(</pre>
    n_species = 10, n_resources = 15,
    trophic_levels = c(6, 3, 1),
    trophic_preferences = list(
        c(rep(1, 5), rep(-1, 5), rep(0, 5)),
        c(rep(0, 5), rep(1, 5), rep(-1, 5)),
        c(rep(0, 10), rep(1, 5))
    )
)
ExampleResources <- c(rep(500, 5), rep(200, 5), rep(50, 5))
tse2 <- simulateConsumerResource(</pre>
    n_{species} = n_{species},
    n_resources = n_resources,
    names_species = letters[1:n_species],
    names_resources = paste0(
        "res", LETTERS[1:n_resources]
    ),
    E = ExampleEfficiencyMatrix,
    x0 = rep(0.001, n\_species),
    resources = ExampleResources,
    growth_rates = rep(1, n_species),
```

simulateGLV 17

```
# error_variance = 0.001,
    t_{end} = 5000, t_{step} = 1
)
# example with trophic priority
n_species <- 4
n_resources <- 6
ExampleE <- randomE(</pre>
    n_{species} = n_{species},
    n_resources = n_resources,
    mean_consumption = n_resources,
    mean\_production = 0
ExampleTrophicPriority <- t(apply(</pre>
    matrix(sample(n_species * n_resources),
        nrow = n_species
    ),
    1, order
))
# make sure that for non-consumables resources for each species,
# the priority is 0 (smaller than any given priority)
ExampleTrophicPriority <- (ExampleE > 0) * ExampleTrophicPriority
tse3 <- simulateConsumerResource(</pre>
    n_species = n_species,
    n_resources = n_resources,
    E = ExampleE,
    trophic_priority = ExampleTrophicPriority,
    t_{end} = 2000
)
```

simulateGLV

Generalized Lotka-Volterra (gLV) simulation

# **Description**

Simulates time series with the generalized Lotka-Volterra model.

## Usage

```
simulateGLV(
  n_species,
  names_species = NULL,
  A = NULL,
  x0 = NULL,
  growth_rates = NULL,
  sigma_drift = 0.001,
  sigma_epoch = 0.1,
  sigma_external = 0.3,
```

18 simulateGLV

```
sigma_migration = 0.01,
epoch_p = 0.001,
t_external_events = NULL,
t_external_durations = NULL,
stochastic = TRUE,
migration_p = 0.01,
metacommunity_probability = NULL,
error_variance = 0,
norm = FALSE,
t_end = 1000,
...
)
```

#### **Arguments**

n\_species Integer: number of species Character: names of species. If NULL, paste0("sp", seq\_len(n\_species)) names\_species is used. (default: names\_species = NULL) matrix: interaction matrix defining the positive and negative interactions be-Α tween n\_species. If NULL, randomA(n\_species) is used. (default: A = NULL) Numeric: initial abundances of simulated species. If NULL, runif(n = n\_species, х0 min = 0, max = 1) is used. (default: x0 = NULL) Numeric: growth rates of simulated species. If NULL, runif(n = n\_species, growth\_rates min = 0, max = 1) is used. (default: growth\_rates = NULL) sigma\_drift Numeric: standard deviation of a normally distributed noise applied in each time step (t\_step) (default: sigma\_drift = 0.001) Numeric: standard deviation of a normally distributed noise applied to random sigma\_epoch periods of the community composition with frequency defined by the epoch\_p parameter (default: sigma\_epoch = 0.1) sigma\_external Numeric: standard deviation of a normally distributed noise applied to userdefined external events/disturbances (default: sigma\_external = 0.3) sigma\_migration Numeric: standard deviation of a normally distributed variable that defines the intensity of migration at each time step (t\_step) (default: sigma\_migration = 0.01)Numeric: the probability/frequency of random periodic changes introduced to epoch\_p the community composition (default:  $epoch_p = 0.001$ ) t\_external\_events Numeric: the starting time points of defined external events that introduce random changes to the community composition (default: t\_external\_events = NULL) t\_external\_durations Numeric: respective duration of the external events that are defined in the 't\_external\_events' (times) and sigma\_external (std). (default: t\_external\_durations = NULL) stochastic Logical: whether to introduce noise in the simulation. If False, sigma drift,

sigma\_epoch, and sigma\_external are ignored. (default: stochastic = FALSE)

simulateGLV 19

```
migration_p
                  Numeric: the probability/frequency of migration from a metacommunity. (de-
                  fault: migration_p = 0.01)
metacommunity_probability
                  Numeric: Normalized probability distribution of the likelihood that species from
                  the metacommunity can enter the community during the simulation. If NULL,
                  rdirichlet(1, alpha = rep(1,n_species)) is used. (default: metacommunity_probability
                  = NULL)
error_variance Numeric: the variance of measurement error. By default it equals to 0, indicating
                  that the result won't contain any measurement error. This value should be non-
                  negative. (default: error_variance = 0)
                  Logical: whether the time series should be returned with the abundances as
norm
                  proportions (norm = TRUE) or the raw counts (default: norm = FALSE) (default:
                  norm = FALSE)
                  Numeric: the end time of the simulation Times, defining the modeled time length
t_{end}
                  of the community. (default: t_end = 1000)
                  additional parameters, see utils to know more.
```

#### **Details**

Simulates a community time series using the generalized Lotka-Volterra model, defined as dx/dt = x(b+Ax), where x is the vector of species abundances, diag(x) is a diagonal matrix with the diagonal values set to x. A is the interaction matrix and b is the vector of growth rates.

#### Value

simulateGLV returns a TreeSummarizedExperiment class object

```
# generate a random interaction matrix
ExampleA \leftarrow randomA(n_species = 4, diagonal = -1)
# run the model with default values (only stochastic migration considered)
tse <- simulateGLV(n_species = 4, A = ExampleA)
# run the model with two external disturbances at time points 240 and 480
# with durations equal to 1 (10 \text{ time steps when t_step by default is } 0.1).
ExampleGLV <- simulateGLV(</pre>
    n_{species} = 4, A = ExampleA,
    t_{external_events} = c(0, 240, 480), t_{external_durations} = c(0, 1, 1)
)
# run the model with no perturbation nor migration
set.seed(42)
tse1 <- simulateGLV(
    n_species = 4, A = ExampleA, stochastic = FALSE,
    sigma_migration = 0
)
```

20 simulateHubbell

```
# run the model with no perturbation nor migration but with measurement error
set.seed(42)
tse2 <- simulateGLV(
    n_species = 4, A = ExampleA, stochastic = FALSE,
    error_variance = 0.001, sigma_migration = 0
)</pre>
```

simulateHubbell

Hubbell's neutral model simulation

# **Description**

Neutral species abundances simulation according to the Hubbell model.

# Usage

```
simulateHubbell(
  n_species,
  M,
  carrying_capacity = 1000,
  k_events = 10,
  migration_p = 0.02,
  t_skip = 0,
  t_end,
  norm = FALSE
)
```

# **Arguments**

| n_species       | integer amount of different species initially in the local community  |
|-----------------|---|
| М               | integer amount of different species in the metacommunity, including those of the local community  |
| carrying_capaci | ity   |
|                 | <pre>integer value of fixed amount of individuals in the local community (default:<br/>carrying_capacity = 1000)</pre>  |
| k_events        | integer value of fixed amount of deaths of local community individuals in each generation (default: $k_{events} = 10$ )   |
| migration_p     | numeric immigration rate: the probability that a death in the local community is replaced by a migrant of the metacommunity rather than by the birth of a local community member (default: migration_p = $0.02$ ) |
| t_skip          | integer number of generations that should not be included in the outputted species abundance matrix. (default: $t_skip = 0$ )   |
| t_end           | integer number of simulations to be simulated   |
| norm            | logical scalar choosing whether the time series should be returned with the abundances as proportions (norm = TRUE) or the raw counts (default: norm = FALSE)   |

simulateHubbellRates 21

#### Value

simulateHubbell returns a TreeSummarizedExperiment class object

#### References

Rosindell, James et al. "The unified neutral theory of biodiversity and biogeography at age ten." Trends in ecology & evolution vol. 26,7 (2011).

## **Examples**

```
tse <- simulateHubbell(
    n_species = 8, M = 10, carrying_capacity = 1000, k_events = 50,
    migration_p = 0.02, t_end = 100
)</pre>
```

simulateHubbellRates Hubbell's neutral model simulation applied to time series

# **Description**

Neutral species abundances simulation according to the Hubbell model. This model shows that losses in society can be replaced either by the birth of individuals or by immigration depending on their probabilities. The specific time between the events of birth or migration is calculated and time effect is considered to determine the next event.

# Usage

```
simulateHubbellRates(
  n_species = NULL,
  x0 = NULL,
  names_species = NULL,
  migration_p = 0.01,
  metacommunity_probability = NULL,
  k_events = 1,
  growth_rates = NULL,
  error_variance = 0,
  norm = FALSE,
  t_end = 1000,
  ...
)
```

#### **Arguments**

```
n_species Integer: number of speciesx0 Numeric: initial species composition. If NULL, rep(100, n_species) is used.
```

22 simulateHubbellRates

```
Character: names of species. If NULL, paste0("sp", seq_len(n_species))
names_species
                  is used. (default: names_species = NULL)
                  Numeric: the probability/frequency of migration from a metacommunity. (de-
migration_p
                  fault: migration_p = 0.01)
metacommunity_probability
                  Numeric: Normalized probability distribution of the likelihood that species from
                  the metacommunity can enter the community during the simulation. If NULL,
                  rdirichlet(1, alpha = rep(1,n_species)) is used. (default: metacommunity_probability
k_events
                  Integer: number of events to simulate before updating the sampling distribu-
                  tions. (default: k_events = 1)
growth_rates
                  Numeric: maximum growth rates(mu) of species. If NULL, rep(1, n_species)
                  is used. (default: growth_rates = NULL)
error_variance Numeric: the variance of measurement error. By default it equals to 0, indicating
                  that the result won't contain any measurement error. This value should be non-
                  negative. (default: error_variance = 0)
                  Logical: whether the time series should be returned with the abundances as
norm
                  proportions (norm = TRUE) or the raw counts (default: norm = FALSE) (default:
                  norm = FALSE)
t_end
                  Numeric: the end time of the simulation Times, defining the modeled time length
                  of the community. (default: t_end = 1000)
                  additional parameters, see utils to know more.
```

## Value

simulateHubbellRates returns a TreeSummarizedExperiment class object

#### References

Rosindell, James et al. "The unified neutral theory of biodiversity and biogeography at age ten." Trends in ecology & evolution vol. 26,7 (2011).

```
set.seed(42)
tse <- simulateHubbellRates(n_species = 5)
miaViz::plotSeries(tse, x = "time")
# no migration, all stochastic birth and death
set.seed(42)
tse1 <- simulateHubbellRates(n_species = 5, migration_p = 0)
# all migration, no stochastic birth and death
set.seed(42)
tse2 <- simulateHubbellRates(
    n_species = 5,
    migration_p = 1,</pre>
```

simulateRicker 23

```
metacommunity_probability = c(0.1, 0.15, 0.2, 0.25, 0.3),
    t_{end} = 20,
    t_store = 200
)
# all migration, no stochastic birth and death, but with measurement errors
set.seed(42)
tse3 <- simulateHubbellRates(</pre>
   n_{species} = 5,
   migration_p = 1,
   metacommunity_probability = c(0.1, 0.15, 0.2, 0.25, 0.3),
    t_{end} = 20,
    t_store = 200,
    error_variance = 100
)
# model with specified inputs
set.seed(42)
tse4 <- simulateHubbellRates(</pre>
   n_{species} = 5,
   migration_p = 0.1,
   metacommunity_probability = c(0.1, 0.15, 0.2, 0.25, 0.3),
   t_{end} = 200,
    t_store = 1000,
   k_{events} = 5,
    growth_rates = c(1.1, 1.05, 1, 0.95, 0.9)
)
```

simulateRicker

Generate time series with the Ricker model

# **Description**

The Ricker model is a discrete version of the generalized Lotka-Volterra model and is implemented here as proposed by Fisher and Mehta in PLoS ONE 2014.

# Usage

```
simulateRicker(
   n_species,
   A,
   names_species = NULL,
   x0 = runif(n_species),
   carrying_capacities = runif(n_species),
   error_variance = 0.05,
   explosion_bound = 10^8,
   t_end = 1000,
   norm = FALSE,
   ...
)
```

24 simulateSOI

#### **Arguments**

n\_species Integer: number of species interaction matrix Character: names of species. If NULL, paste0("sp", seq\_len(n\_species)) names\_species is used. (default: names\_species = NULL) x0 Numeric: initial abundances of simulated species. If NULL, runif(n = n\_species, min = 0, max = 1) is used. carrying\_capacities numeric carrying capacities. If NULL, runif(n = n\_species, min = 0, max = 1) is used. error\_variance Numeric: the variance of measurement error. By default it equals to 0, indicating that the result won't contain any measurement error. This value should be nonnegative. (default: error\_variance = 0.05) explosion\_bound numeric value of boundary for explosion (default: explosion\_bound = 10^8) t\_end integer number of simulations to be simulated logical scalar returning normalised abundances (proportions in each generation) norm (default: norm = FALSE)

#### Value

simulateRicker returns a TreeSummarizedExperiment class object

#### References

Fisher & Mehta (2014). Identifying Keystone Species in the Human Gut Microbiome from Metagenomic Timeseries using Sparse Linear Regression. PLoS One 9:e102451

additional parameters, see utils to know more.

# **Examples**

```
A <- powerlawA(10, alpha = 1.01)
tse <- simulateRicker(n_species = 10, A, t_end = 100)
```

simulateS0I

Self-Organised Instability model (SOI) simulation

# Description

Generate time-series with The Self-Organised Instability (SOI) model. Implements a K-leap method for accelerating stochastic simulation.

simulateSOI 25

# Usage

```
simulateSOI(
    n_species,
    x0 = NULL,
    names_species = NULL,
    carrying_capacity = 1000,
    A = NULL,
    k_events = 5,
    t_end = 1000,
    metacommunity_probability = runif(n_species, min = 0.1, max = 0.8),
    death_rates = runif(n_species, min = 0.01, max = 0.08),
    norm = FALSE
)
```

# **Arguments**

|                           | n_species       | Integer: number of species   |
|---------------------------|-----------------|--|
|                           | x0              | a vector of initial community abundances If (default: $x0 = NULL$ ), based on migration rates  |
|                           | names_species   | Character: names of species. If NULL, paste0("sp", seq_len(n_species)) is used. (default: names_species = NULL)  |
|                           | carrying_capaci | ty   |
|                           |                 | integer community size, number of available sites (individuals)  |
|                           | A               | matrix: interaction matrix defining the positive and negative interactions between n_species. If NULL, powerlawA(n_species) is used. (default: $A = NULL$ )  |
|                           | k_events        | integer number of transition events that are allowed to take place during one leap. (default: k_events = 5). Higher values reduce runtime, but also accuracy of the simulation.  |
|                           | t_end           | Numeric: the end time of the simulation, defining the modeled time length of the community. (default: t_end = 1000)  |
| metacommunity_probability |                 |  |
|                           |                 | Numeric: Normalized probability distribution of the likelihood that species from the metacommunity can enter the community during the simulation. By default, $runif(n\_species, min = 0.1, max = 0.8)$ is used. (default: metacommunity_probability = $runif(n\_species, min = 0.1, max = 0.8)$ ) |
|                           | death_rates     | Numeric: death rates of each species. By default, runif(n_species, min = 0.01, max = 0.08) is used. (default: death_rates = runif(n_species, min = 0.01, max = 0.08))  |
|                           | norm            | logical scalar indicating whether the time series should be returned with the abundances as proportions (norm = TRUE) or the raw counts (default: norm = FALSE)  |
|                           |                 |  |

# Value

simulateSOI returns a TreeSummarizedExperiment class object

#### **Examples**

```
# Generate interaction matrix
A <- miaSim::powerlawA(10, alpha = 1.2)
# Simulate data from the SOI model
tse <- simulateSOI(
    n_species = 10, carrying_capacity = 1000, A = A,
    k_events = 5, x0 = NULL, t_end = 150, norm = TRUE
)</pre>
```

simulateStochasticLogistic

Stochastic Logistic simulation

# **Description**

Simulates time series with the (stochastic) logistic model

## Usage

```
simulateStochasticLogistic(
  n_species,
 names_species = NULL,
 growth_rates = NULL,
  carrying_capacities = NULL,
  death_rates = NULL,
 x0 = NULL,
  sigma_drift = 0.001,
  sigma_epoch = 0.1,
  sigma_external = 0.3,
  sigma_migration = 0.01,
  epoch_p = 0.001,
  t_external_events = NULL,
  t_external_durations = NULL,
 migration_p = 0.01,
 metacommunity_probability = NULL,
  stochastic = TRUE,
  error_variance = 0,
  norm = FALSE,
  t_{end} = 1000,
)
```

# **Arguments**

n\_species Integer: number of species

names\_species Character: names of species. If NULL, paste0("sp", seq\_len(n\_species)) is used. (default: names\_species = NULL) Numeric: growth rates of simulated species. If NULL, runif(n = n\_species, growth\_rates min = 0.1, max = 0.2) is used. (default: growth\_rates = NULL) carrying\_capacities Numeric: The max population of species supported in the community. If NULL, runif(n = n\_species, min = 1000, max = 2000) is used. (default: carrying\_capacities = NULL) death\_rates Numeric: death rates of each species. If NULL, runif(n = n\_species, min = 0.0005, max = 0.0025) is used. (default: death\_rates = NULL) х0 Numeric: initial abundances of simulated species. If NULL, runif(n = n\_species, min = 0.1, max = 10) is used. (default: x0 = NULL) sigma\_drift Numeric: standard deviation of a normally distributed noise applied in each time step (t\_step) (default: sigma\_drift = 0.001) sigma\_epoch Numeric: standard deviation of a normally distributed noise applied to random periods of the community composition with frequency defined by the epoch\_p parameter (default: sigma\_epoch = 0.1) sigma\_external Numeric: standard deviation of a normally distributed noise applied to userdefined external events/disturbances (default: sigma\_external = 0.3) sigma\_migration Numeric: standard deviation of a normally distributed variable that defines the intensity of migration at each time step (t\_step) (default: sigma\_migration = 0.01)Numeric: the probability/frequency of random periodic changes introduced to epoch\_p the community composition (default:  $epoch_p = 0.001$ ) t\_external\_events Numeric: the starting time points of defined external events that introduce random changes to the community composition (default: t\_external\_events = NULL) t\_external\_durations Numeric: respective duration of the external events that are defined in the 't\_external\_events' (times) and sigma\_external (std). (default: t\_external\_durations = NULL) Numeric: the probability/frequency of migration from a metacommunity. (demigration\_p fault: migration\_p = 0.01) metacommunity\_probability Numeric: Normalized probability distribution of the likelihood that species from the metacommunity can enter the community during the simulation. If NULL, rdirichlet(1, alpha = rep(1, n\_species)) is used. (default: metacommunity\_probability = NULL) stochastic Logical: whether to introduce noise in the simulation. If False, sigma\_drift,

sigma\_epoch, and sigma\_external are ignored. (default: stochastic = TRUE)

that the result won't contain any measurement error. This value should be non-

error\_variance Numeric: the variance of measurement error. By default it equals to 0, indicating

negative. (default: error\_variance = 0)

norm

Logical: whether the time series should be returned with the abundances as proportions (norm = TRUE) or the raw counts (default: norm = FALSE) (default: norm = FALSE)

T\_end

Numeric: the end time of the simulationTimes, defining the modeled time length of the community. (default: t\_end = 1000)

additional parameters, see utils to know more.

#### **Details**

The change rate of the species was defined as dx/dt = b\*x\*(1-(x/k))\*rN - dr\*x, where b is the vector of growth rates, x is the vector of initial species abundances, k is the vector of maximum carrying capacities, rN is a random number ranged from 0 to 1 which changes in each time step, dr is the vector of constant death rates. Also, the vectors of initial dead species abundances can be set. The number of species will be set to 0 if the dead species abundances surpass the alive species abundances.

#### Value

simulateStochasticLogistic returns a TreeSummarizedExperiment class object

```
# Example of logistic model without stochasticity, death rates, or external
# disturbances
set.seed(42)
tse <- simulateStochasticLogistic(</pre>
   n_{species} = 5,
    stochastic = FALSE, death_rates = rep(0, 5)
)
# Adding a death rate
set.seed(42)
tse1 <- simulateStochasticLogistic(</pre>
   n_{species} = 5,
    stochastic = FALSE, death_rates = rep(0.01, 5)
)
# Example of stochastic logistic model with measurement error
set.seed(42)
tse2 <- simulateStochasticLogistic(</pre>
   n_{species} = 5,
    error_variance = 1000
)
# example with all the initial parameters defined by the user
set.seed(42)
tse3 <- simulateStochasticLogistic(</pre>
   n_{species} = 2,
    names_species = c("species1", "species2"),
    growth_rates = c(0.2, 0.1),
    carrying_capacities = c(1000, 2000),
```

```
death_rates = c(0.001, 0.0015),
    x0 = c(3, 0.1),
    sigma_drift = 0.001,
    sigma_epoch = 0.3,
    sigma_external = 0.5,
    sigma_migration = 0.002,
    epoch_p = 0.001,
    t_{external_events} = c(100, 200, 300),
    t_{external_durations} = c(0.1, 0.2, 0.3),
    migration_p = 0.01,
    metacommunity_probability = miaSim::.rdirichlet(1, alpha = rep(1, 2)),
    stochastic = TRUE,
    error_variance = 0,
    norm = FALSE, # TRUE,
    t_{end} = 400,
    t_{start} = 0, t_{step} = 0.01,
    t_store = 1500
)
```

# **Index**

```
* internal
    .simulationTimes, 7
.applyInterType, 2
. {\tt estimateAFromSimulations}, 3
.eventTimes, 4
.getInteractions, 5
.isPosInt, 5
.rdirichlet, 6
.replaceByZero, 6
.simulationTimes, 7
powerlawA, 7
randomA, 8
randomE, 11
simulateConsumerResource, 13
simulateGLV. 17
simulateHubbell, 20
simulateHubbellRates, 21
simulateHubbellRates,numeric-method
        (simulateHubbellRates), 21
simulateHubbellRates-numeric
        (simulateHubbellRates), 21
simulateRicker, 23
simulateSOI, 24
simulateStochasticLogistic, 26
utils, 15, 19, 22, 24, 28
```