

Package ‘samovaR’

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Type Package

Title R package for generating model metagenomes with specified properties

Version 0.5

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```
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```

Description There is a fundamental problem in modern ***metagenomics***: there are huge differences between methodological approaches that strongly influence the results, while remaining outside the attention of researchers. We propose an approach that utilizes de novo generation of the artificial metagenomes - ‘SamovaR’.

URL <https://github.com/dsmutin/samovar/>

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Encoding UTF-8

LazyData true

Imports tidyverse,

```
plotly,
httr,
jsonlite,
xml2,
tsne,
cluster,
Matrix,
shiny,
here,
methods,
scclust
```

Roxygen list(markdown = TRUE)

RoxygenNote 7.3.2

Suggests ggnewscale,

```
knitr,
rmarkdown,
testthat (>= 3.0.0)
```

VignetteBuilder knitr

Config/testthat/edition 3

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build_samovar	<i>Build samovar object</i>
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Description

Samovar network is a 2D-oriented graph with metadata and abundances of species per sample. Oriented graph could be used for network prediction, or for better generation some network could be used as initial (to be implemented) For better understanding of building database and using it in generation, visit github source

Usage

```
build_samovar(
  samovar_data,
  dist_function = function(x) dist(x),
  network = F,
  k_means = F,
  min_cluster_size = F,
  plot_log = T
)
```

Arguments

samovar_data	samovar data after preprocessing stages
network	FALSE or graph that can be used for generation. To be implemented
plot_log	Logical or path for log plots output
distance_function	function used for measuring distances between species based on samples

min_min_cluster_size
FALSE or minimum number of species per cluster

max_min_cluster_size
FALSE or minimum number of species per cluster

concotion_pour	<i>Build samovar object</i>
----------------	-----------------------------

Description

Samovar network is a 2D-oriented graph with metadata and abundances of species per sample. Oriented graph could be used for network prediction, or for better generation some network could be used as initial (to be implemented) For better understanding of building database and using it in generation, visit github source

Usage

```
concotion_pour(
  samovar_data,
  inner_method = "glm",
  inter_method = "glm",
  inner_model = "gaussian",
  inter_model = "gaussian",
  minimal_cluster = 2,
  probability_calculation = "oriented",
  cluster_connection = "mean"
)
```

Arguments

samovar_data	samovar data after preprocessing stages
inner_method	Character, glm, other to be implemented (bootstrap, bsPCA)
inter_method	Character, glm, other to be implemented (bootstrap, bsPCA)
inner_model	Character, model processed by glm(). For glm mode only. quasipoisson by default
inter_model	Character, model processed by glm(). For glm mode only. quasipoisson by default
cluster_connection	Character (mean, median), or function. The way of cluster connection. If function, way of summarize all samples of species cluster
network	FALSE or graph that can be used for generation. To be implemented
cooccurrence	Character, co-occurrence calculation. If "simple", calculated as: $P(A B) = \text{sum}(A \& B) / \text{sum}(A B)$. If "oriented", calculated as $P(A B) = P(A \& B B)$ If "compositional", calculated as $P(A B) = P(A \& B B)$, and than sampled one of represented conditions of occurence

Examples

```
# download data
teatree <- GMrepo_type2data(number_to_process = 2000)

# filter
tealeaves <- teatree %>%
  teatree_trim(treshhold_species = 3, treshhold_samples = 3, treshhold_amount = 10^(-3))

# normalizing
## if you build teatree by your own, rescaling stage when building via teatree$rescale() or assigning teatree$mi
## good approximation to normal distribution is required for glm generating methods
teabag <- tealeaves %>%
  tealeaves_pack(normalization_function = function(x) log10(x+1))

# clustering
concotion <- teabag %>%
  teabag_brew(min_cluster_size = 4, max_cluster_size = 6)
# remember: if you want to refilter, it is better to re-do welding stage to avoid crashes in future!

# building samovar
samovar <- concotion %>%
  concotion_pour()
```

GMrepo_run	<i>GMrepo run data class</i>
------------	------------------------------

Description

GMrepo run data class

Slots

metadata metadata DataFrame
run character

GMrepo_run2data	<i>Get data from GMrepo_run object</i>
-----------------	--

Description

Get data from GMrepo_run object

Usage

```
GMrepo_run2data(  
  run,  
  number_to_out = F,  
  at_level = "species",  
  QC_filter = "QCStatus"  
)
```

Arguments

number_to_out	False by default, maximum number of obtained data
at_level	"species" by default. level to obtain classification from GMrepo
QC_filter	QCStatus by default. Perform auto QC filtering based on metadata column, or False for no checking.
runs	GMrepo_run object got by GMrepo_type2run or created by user with <code>new('GMrepo_run', metadata = data.frame(), run = run_list)</code>

Examples

```
# get data from GMrepo
data_GMrepo <- GMrepo_type2data(mesh_ids = "D006262", number_to_process = 1000)

# equal to:
run_GMrepo <- GMrepo_type2run(mesh_ids = "D006262", number_to_process = 1000)
data_GMrepo <- GMrepo_run2data(run_GMrepo)

# filter runs before obtaining data (OOP updating data!)
run_GMrepo$filter("checking", 1)

# view
data_GMrepo

# access to metadata
data_GMrepo$run

# access to data
data_GMrepo$data

# access to runs
data_GMrepo$run

# access to taxa
data_GMrepo$species
```

GMrepo_type2data	<i>Get data from GMrepo</i>
------------------	-----------------------------

Description

Wrapper around GMrepo_type2run and GMrepo_run2data functions

Usage

```
GMrepo_type2data(
  mesh_ids = c("D006262"),
  number_to_process = F,
  number_to_out = F,
  at_level = "species",
  QC_filter = "QCStatus"
)
```

Arguments

mesh_ids	Character. All types of meshID to use. List of relations between meshID and phenotype could be obtained using GMrepo_meshID(). Health meshID by default
number_to_process	False by default, or maximum number of runs per meshID
number_to_out	False by default, maximum number of obtained data
at_level	"species" by default. level to obtain classification from GMrepo
QC_filter	QCStatus by default. Perform auto QC filtering based on metadata column, or False for no checking.

Examples

```
# get data from GMrepo
data_GMrepo <- GMrepo_type2data(mesh_ids = "D006262", number_to_process = 1000)

# equal to:
run_GMrepo <- GMrepo_type2run(mesh_ids = "D006262", number_to_process = 1000)
data_GMrepo <- GMrepo_run2data(run_GMrepo)

# filter runs before obtaining data (OOP updating data!)
run_GMrepo$filter("checking", 1)

# view
data_GMrepo

# access to metadata
data_GMrepo$run

# access to data
data_GMrepo$data

# access to runs
data_GMrepo$run

# access to taxa
data_GMrepo$species
```

GMrepo_type2run	<i>Get runs from GMrepo by meshID</i>
-----------------	---------------------------------------

Description

Get runs from GMrepo by meshID

Usage

```
GMrepo_type2run(mesh_ids = c("D006262"), number_to_process = F)
```

Arguments

mesh_ids Character. All types of meshID to use. List of relations between meshID and phenotype could be obtained using GMrepo_meshID()

number_to_process False by default, or maximum number of runs per meshID

Examples

```
# get data from GMrepo
data_GMrepo <- GMrepo_type2data(mesh_ids = "D006262", number_to_process = 1000)

# equal to:
run_GMrepo <- GMrepo_type2run(mesh_ids = "D006262", number_to_process = 1000)
data_GMrepo <- GMrepo_run2data(run_GMrepo)

# filter runs before obtaining data (OOP updating data!)
run_GMrepo$filter("checking", 1)

# view
data_GMrepo

# access to metadata
data_GMrepo$run

# access to data
data_GMrepo$data

# access to runs
data_GMrepo$run

# access to taxa
data_GMrepo$species
```

log_plot*Print a log plot*

Description

Print a log plot

Usage

```
log_plot(plot_log, postfix, gg, mode = "ggplot")
```

minmaxscale	<i>Misc functions</i>
-------------	-----------------------

Description

Misc functions

Usage

```
minmaxscale(x)
```

progress_function	<i>Progress bar</i>
-------------------	---------------------

Description

Progress bar

Usage

```
progress_function(iters)
```

read.abundance	<i>Build samovar data object from file or environment</i>
----------------	---

Description

Build samovar data object from file or environment

Usage

```
read.abundance(data, metadata, ...)
```

Arguments

data	Data.frame or path to abundance file. Row names is using as species list, column names as sample list. Unique names required
metadata	Data.frame or path to metadata file
...	Parameters processed by read.table()

read.samovar	<i>Read samovar data frame from file</i>
--------------	--

Description

Prints 'Hello, world!'.

Usage

```
hello()
```

Examples

```
hello()
```

samovar_base	<i>samovar base class</i>
--------------	---------------------------

Description

samovar base class

Slots

samovar_base samovar_data object

method method to obtain samovar_base

inner_cluster_graph_method list of graphs in matrix form of inner cluster connections

inter_cluster_graph_method list of graphs in matrix form of inter cluster connections

inner_cluster_graph_prob list of co-occurrence probabilities in matrix form of inner cluster members

inter_cluster_graph_prob list of co-occurrence probabilities in matrix form between clusters

properties concotion_pour() properties

samovar_boil	<i>Generate artificial data</i>
--------------	---------------------------------

Description

Use pre-built samovar_data with its parameters

Usage

```
samovar_boil(
  samovar_base,
  N = 1,
  init_sp = F,
  init_ab = F,
  avoid_zero_generations = T,
  seed = 42
)
```

Arguments

samovar_base	samovar data after preprocessing and building stages
N	number of artificial samples to generate
init_sp	species vector for initializing data generation, or FALSE for usage most common taxa, auto for choosing random taxa
init_ab	species amount vector (values from 0 to 1) for initializing data generation, or FALSE for mean initial taxa assignment, or auto for usage from known edf for each species from init_sp
avoid_zero_generations	logical, avoid zero-based generations or not. FALSE might results in under-distributed communities, while TRUE in over-represented with species from different clusters possibly come from different samples groups
seed	initial seed for the seeds generation

Examples

```
# download and prepare data
samovar <- GMrepo_type2data(number_to_process = 2000) %>%
  teatree_trim(treshhold_species = 3, treshhold_samples = 3, treshhold_amount = 10^(-3)) %>%
  tealeaves_pack(normalization_function = function(x) log10(x+1)) %>%
  teabag_brew(min_cluster_size = 4, max_cluster_size = 6) %>%
  concotion_pour()

# generate
new_data <- samovar %>%
  samovar_boil(n = 100)
```

samovar_data	<i>samovar data class</i>
--------------	---------------------------

Description

samovar data class

Slots

description metadata DataFrame
 data DataFrame with species abundances. No NA pass
 run character, runs
 species character, runs
 normalization_function normalization function for samples
 reverse_normalization_function reverse normalization function
 min_value minimal value after scaling
 max_value maximal value after scaling
 cluster character vector, enumerated clusters for each species
 cluster_size named numeric, cluster sizes per cluster

samovar_run	<i>Samovar run data class</i>
-------------	-------------------------------

Description

Samovar run data class

Slots

metadata metadata DataFrame
 data data
 run character, samle IDs

Methods

export(Class) Returns the result of coercing the object to Class. No effect on the object itself.

teabag_brew	<i>Build samovar object</i>
-------------	-----------------------------

Description

Samovar network is a 2D-oriented graph with metadata and abundances of species per sample. Oriented graph could be used for network prediction, or for better generation some network could be used as initial (to be implemented) For better understanding of building database and using it in generation, visit github source

Usage

```
teabag_brew(
  samovar_data,
  dist_function = function(x) dist(x),
  network = F,
  min_cluster_size = 10,
  max_cluster_size = 100,
  plot_log = T
)
```

Arguments

network	FALSE or graph that can be used for generation. To be implemented
min_cluster_size	FALSE or minimum number of species per cluster
max_cluster_size	FALSE or minimum number of species per cluster
plot_log	Logical or path for log plots output
data	samovar data after preprocessing stages
distance_function	function used for measuring distances between species based on samples

tealeaves_pack	<i>Scale species abundances</i>
----------------	---------------------------------

Description

Scale species abundances

Usage

```
tealeaves_pack(
  samovar_data,
  normalization_function = function(x) log10(x + 1),
  plot_log = T
)
```

Arguments

samovar_data Samovar data object to rescale
 normalization_function Function using for rescaling
 plot_log Logical or path for log plots output

Examples

```

# download data
teatree <- GMrepo_type2data(number_to_process = 2000)

# filter
tealeaves <- teatree %>%
  teatree_trim(treshhold_species = 3, treshhold_samples = 3, treshhold_amount = 10^(-3))

# normalizing
## if you build teatree by your own, rescaling stage when building via teatree$rescale() or assigning teatree$mi
## good approximation to normal distribution is required for glm generating methods
teabag <- tealeaves %>%
  tealeaves_pack(normalization_function = function(x) log10(x+1))

# clustering
concotion <- teabag %>%
  teabag_brew(min_cluster_size = 4, max_cluster_size = 6)
# remember: if you want to refilter, it is better to re-do welding stage to avoid crashes in future!

# building samovar
samovar <- concotion %>%
  concotion_pour()
  
```

teatree_trim	<i>Filter species and samples from samovar_data object</i>
--------------	--

Description

Filter species and samples from samovar_data object

Usage

```

teatree_trim(
  samovar_data,
  metadata_filter = F,
  treshhold_amount = 10^(-5),
  treshhold_samples = 1,
  treshhold_species = 1,
  drop_species = F,
  drop_unclassified = T
)
  
```

Arguments

samovar_data Samovar data object to filter
metadata_filter False, character or data.frame with 2 columns: first contain metadata names for filtering, and second values per column
threshhold_amount Minimum value to conclude as not the noise.
threshhold_samples Minimum number of representing samples to keep species.
threshhold_species Minimum number of representing species to keep samples.
drop_unclassified Drop unknown and unclassified ranks. True by default

Examples

```

# download data
teatree <- GMrepo_type2data(number_to_process = 2000)

# filter
tealeaves <- teatree %>%
  teatree_trim(treshhold_species = 3, treshhold_samples = 3, treshhold_amount = 10^(-3))

# normalizing
## if you build teatree by your own, rescaling stage when building via teatree$rescale() or assigning teatree$mi
## good approximation to normal distribution is required for glm generating methods
teabag <- tealeaves %>%
  tealeaves_pack(normalization_function = function(x) log10(x+1))

# clustering
concotion <- teabag %>%
  teabag_brew(min_cluster_size = 4, max_cluster_size = 6)
# remember: if you want to refilter, it is better to re-do welding stage to avoid crashes in future!

# building samovar
samovar <- concotion %>%
  concotion_pour()

```

viz_composition

*Visualize composition***Description**

Visualize composition

Usage

```

viz_composition(
  data,
  reord_samples = "fpc",
  reord_species = "amount",

```

```

    type = "column",
    top = 15,
    interactive = F,
    ggplot_add = F,
    bottom_legend = F
  )

```

Arguments

data	data.frame with dimensions of species * samples, or samovar objects: samovar_data, samovar_base, samovar_run or GMrepo_run (with data)
reord_samples	character, fpc, fpc_scaled, hcl, amount, tsne, or none reorder of samples on plot
reord_species	character, same for reord_samples
type	character, column or tile for composition visualize, or donut (to implement) for mean composition visualization
top	integer, number of top-represented taxa to show, or FALSE to show all
interactive	logical. ggplot or plotly object to return
ggplot_add	functions to add to ggplot object, or FALSE.
bottom_legend	vector length of samples to show on plot as a color legend, or FALSE

Examples

```

# Download data
teatree <- GMrepo_type2data(number_to_process = 1000)

#Composition
viz_composition(teatree)

```

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