Package 'TemporalGSSA'

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Type Package

Title Outputs Temporal Profile of Molecules from Stochastic Simulation
Algorithm Generated Datasets

Version 1.0.1

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Description The data that is generated from independent and consecutive 'Gille-
spieSSA' runs for a generic biochemical network
is formatted as rows and constitutes an observation. The first column of each row is the com-
puted timestep for each run. Subsequent
columns are used for the number of molecules of each participating molecu-
lar species or ``metabolite'' of a generic biochemical network.
In this way 'TemporalGSSA', is a wrapper for the R-
package 'GillespieSSA'. The number of observations must be at least 30.
This will generate data that is statistically significant. 'TemporalGSSA', trans-
forms this raw data into a simulation time-dependent and metabolite-specific
trial. Each such trial is defined as a set of linear models (n >= 30) between a timestep and num-
ber of molecules for a metabolite. Each linear model
is characterized by coefficients such as the slope, arbitrary constant, etc. The user must en-
ter an integer from 1-4.
These specify the statistical modality utilized to compute a representative timestep (mean, me-
dian, random, all).
These arguments are mandatory and will be checked. Whilst, the numeric indicator ``0'' indi-
cates suitability,
``1'' prompts the user to revise and re-
enter their data. An optional logical argument controls the output to the
console with the default being ``TRUE'' (curtailed) whilst ``FALSE'' (verbose). The coeffi-
cients of each linear model are averaged (mean slope, mean constant)
and are incorporated into a metabolite-specific linear regression model as the dependent vari-
able. The independent variable is the representative timestep
chosen previously. The generated data is the imputed molecule number for an in silico experi-
ment with (n >=30)
observations. These steps can be replicated with multiple set of observations. The gener-
ated ``technical

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replicates" can be statistically evaluated (mean, standard deviation) and will constitute simula-
tion time-dependent molecules for each metabolite.
For SSA-
generated datasets with varying simulation times 'TemporalGSSA' will generate a simulation time-
dependent trajectory for each metabolite
of the biochemical network under study. The relevant publication with the mathematical deriva-
tion of the algorithm is
(2022, Journal of Bioinformatics and Computational Biol-
ogy) <doi:10.1142/S0219720022500184>. The algorithm has been deployed in the follow-
ing publications
(2021, Heliyon) <doi:10.1016/j.heliyon.2021.e07466> and (2016, Journal of Theoretical Biol-
ogy) <doi:10.1016/j.jtbi.2016.07.002>.

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Encoding UTF-8

Depends stats

Suggests testthat (>= 3.0.0)

RoxygenNote 7.1.2

Config/testthat/edition 3

NeedsCompilation no

Repository CRAN

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Contents

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calculate_TemporalGSSA

*calculate_TemporalGSSA() This is the main function of the package
'TemporalGSSA'.*

Description

'TemporalGSSA', may be considered a wrapper for the R-package 'GillespieSSA'. The formatted
data generated by consecutive runs of 'GillespieSSA' for molecules of a generic biochemical net-
work will generate a dataset of randomly chosen timesteps along with changes to the corresponding
number of molecules. This constitutes a set observations for a specific simulation time.

Usage

```
calculate_TemporalGSSA(data, type, out)
```

Arguments

data	Formatted data from the output of consecutive 'GillespieSSA' runs. This is a mandatory argument.
type	A mandatory integer argument that indicates the statistic that will be used to compute the representative timestep for a set of observations. Here: "1" is the MEAN, "2" is the MEDIAN, "3" is a random choice and "4" is ALL
out	An optional logical argument that control the console output with default being "TRUE" Here, TRUE curtails the output while FALSE allows the verbose output of all the coefficents .

Details

The temporal profile of a metabolite is a pre-requisite to comprehend its behaviour in vivo.

This is accomplished by transforming the raw formatted data into a metabolite-specific trial. Each such trial is defined as a set of linear models (n >= 30) between a timestep and number of molecules for a metabolite. The coefficients of these models (slope, constant) are averaged and incorporated into a metabolite-specific linear regression model. The independent variable is a representative timestep and is user-dependent. The generated data is an imputed number of molecules for each metabolite, is dependent on the simulation time and is defined as a "technical replicate".

The above steps are easily repeated with additional SSA-runs (n >=30) and will generate sets of "technical replicates". These can be statistically evaluated (mean, standard deviation) and will constitute the simulation time-dependent number of molecules for a particular metabolite. For varying simulation times 'TemporalGSSA' will generate a metabolite-specific and simulation time-dependent trajectory.

Value

code A numerically encoded ('0', success; '1', no success) text message to the user indicating the outcome of "TemporalGSSA".

The examples listed below can be run directly from the console as example("calculate_TemporalGSSA")

Examples

```
calculate_TemporalGSSA(valid,1)
calculate_TemporalGSSA(valid,4)
calculate_TemporalGSSA(nvalid,2)
```

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check_TemporalGSSA	*check_TemporalGSSA()*

Description

This function of the package 'TemporalGSSA' checks whether the user-defined data is suitable for further processing.

Usage

```
check_TemporalGSSA(data, type)
```

Arguments

data   Formatted data from the output of a GillespieSSA run This is a mandatory argument.

type   A mandatory integer argument that indicates the statistic to be used to compute the representative timestep for a set of observations. Here: "1" is the MEAN, "2" is the MEDIAN, "3" is a random choice, "4" ALL

Details

The number of observations must be at least 30 (consecutive runs of 'GillespieSSA') to generate data that is statistically significant. The user must also enter a choice that specifies the statistical modality utilized to compute a representative timestep (1, mean; 2, median; 3, random; 4, all). Both arguments are mandatory.

Value

flag A numeric indicator of the suitability of the user-defined input data for further computations.

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