

Package: TemporalGSSA (via r-universe)

August 28, 2024

Type Package

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

Version 1.0.1

Author Siddhartha Kundu

Maintainer Siddhartha Kundu <siddhartha_kundu@aiims.edu>

Description The data that is generated from independent and consecutive 'GillespieSSA' runs for a generic biochemical network is formatted as rows and constitutes an observation. The first column of each row is the computed timestep for each run. Subsequent columns are used for the number of molecules of each participating molecular 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', transforms this raw data into a simulation time-dependent and metabolite-specific trial. Each such trial is defined as a set of linear models ($n \geq 30$) between a timestep and number of molecules for a metabolite. Each linear model is characterized by coefficients such as the slope, arbitrary constant, etc. The user must enter an integer from 1-4. These specify the statistical modality utilized to compute a representative timestep (mean, median, random, all). These arguments are mandatory and will be checked. Whilst, the numeric indicator ``0" indicates 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 coefficients of each linear model are averaged (mean slope, mean constant) and are incorporated into a metabolite-specific linear regression model as the dependent variable. The independent variable is the representative timestep chosen previously. The generated data is the imputed molecule number for an in silico experiment with ($n \geq 30$) observations. These steps can be replicated with

multiple set of observations. The generated "technical replicates" can be statistically evaluated (mean, standard deviation) and will constitute simulation 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 derivation of the algorithm is (2022, Journal of Bioinformatics and Computational Biology) <doi:10.1142/S0219720022500184>. The algorithm has been deployed in the following publications (2021, Heliyon) <doi:10.1016/j.heliyon.2021.e07466> and (2016, Journal of Theoretical Biology) <doi:10.1016/j.jtbi.2016.07.002>.

License GPL-3

Encoding UTF-8

Depends stats

Suggests testthat (>= 3.0.0)

RoxygenNote 7.1.2

Config/testthat/edition 3

NeedsCompilation no

Repository CRAN

Date/Publication 2022-10-09 14:10:02 UTC

Contents

calculate_TemporalGSSA	2
check_TemporalGSSA	3
Index	5

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 network 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 coefficients .

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 ($n \geq 30$) 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 ($n \geq 30$) 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)
```

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.

Index

calculate_TemporalGSSA, 2
check_TemporalGSSA, 3