Package 'TemporalGSSA'

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Type Package

Title Outputs Temporal Profile of Molecules Undergoing Stochastic Simulations

Version 1.0.0

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Description

The data that is generated from consecutive 'GillespieSSA' runs for a generic biochemical network is formatted as ``rows''. The first column of each row constitutes the computed timestep. Subsequent
columns are used for the participating molecules of a generic biochemical network. In this way 'TemporalGSSA',
may be considered a wrapper for the R-
package 'GillespieSSA'. The number of observations must be at least 30.
This will generate data that is statistically significant. The user must also 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 temporal profile of a molecule
is necessary to comprehend its' behaviour within the cell. This is accomplished by selecting a representative
timestep for a set of observations or consecutive runs (n >= 30). A linear model of the numbers of each molecule is
created with the associated timestep from these observations. The coefficients of this model (slope, constant) are then
incorporated into a second linear regression model. Here, the independent variable is the representative timestep
chosen previously. The generated data is the imputed molecule number for an in silico experiment with (n >=30)
observations. These steps can be replicated with multiple set of observations or runs. The generated ``technical

replicates" can be averaged and will constitute the time-
dependent data point of each molecule for a particular simulation
time. For varying simulation times these data will generate time-
dependent trajectories for each molecule
of the biochemical network under study. The algorithm has been deployed effectively in previous publications Kundu, S
(2021, Heliyon) <doi:10.1016/j.heliyon.2021.e07466> and (2016, Journal of Theoretical Biology) <doi:10.1016/j.jtbi.2016.07.002>.

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Depends stats

Suggests testthat (>= 3.0.0)

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NeedsCompilation no

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R topics documented:

`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 timesteps along with changes to the corresponding number of molecules.

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 molecule is a pre-requisite to comprehend its' behaviour in vivo.

This is accomplished by selected a representative timestep for a set of observations or consecutive runs (n >= 30). A linear model of the numbers of each molecule is created with the assocated timestep from these observations. The coefficients of this model (slope, constant) are then incorporated into a second linear regression model.

Here, the independent variable is the representative timestep. The generated data, i.e., the imputed molecule number for an in-silico experiment with n >=30 observations.

This can be replicated with one or more sets of observations or runs. These "technical replicates" can be averaged and will constitute the time-dependent data point of each molecule for a particular simulation time. For varying simulation times these data will generate time-dependent trajectories for each molecule of the biochemical network under study.

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 (consective 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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