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Type Package

Title S-system parameter estimation method

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Description This package can optimize the parameter in S-system models given time series data

License GPL-2

LazyLoad yes

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SPEM-package *S-system parameter estimation method package*

Description

The function in this package allows for the computation of parameters in the n-gene S-system from time series data.

Details

Package:	SPEM
Type:	Package
Version:	1.0
Date:	2013-01-13
License:	GPL-2
LazyLoad:	yes

Author(s)

Yang, X-Y, Dent, J. E. and Nardini, C.

Maintainer: Xinyi Yang <yangxinyi@picb.ac.cn>

row_optimize *Calculate parameters for one row*

Description

This function calculates parameters for a single row in the expression data. If a large-size dataset will be calculated, this function is recommended.

Usage

```
## S4 method for signature 'ExpressionSet'
row_optimize(TS_eSet,S,beta, sparsity = 0.2, lbH = -3, ubH = 3, lbB = 0, ubB = 10)
```

Arguments

TS_eSet	Time series data in ExpressionSet class assayData: Matrix with n metabolite in row and m time points in column. phenoData: Dataframe includes label "time", which represents the time points.
S	Slope of the row you want to calculated. You can either input a vector with length equal to the rows of assayData of TS_eSet, or use s_diff function in this package to calculate it.
beta	Initial beta.
sparsity	A threshold used to control the sparsity of reconstructed matrix. Values whose absolute value smaller than sparsity will be set to zero.
lbH	Lower boundary value of h.
ubH	Upper boundary value of h.
lbB	Lower boundary value of beta.
ubB	Upper boundary value of beta.

Details

In this SPEM package, we aim to reconstruct gene networks from time-series expression data using the S-system model. The input dataset should be as an ExpressionSet data container, describing, in assayData, expression data for n genes (rows) and m time points (columns), along with a vector of length m, which records the exact values of time points, thus showing the sample intervals in phenoData. SPEM will calculate the parameters alpha, g, beta and h of the S-system function set that best fits the dataset.

In this function, user can calculate one row at a time. This function offers a parallel calculation option for users.

Value

This function return a vector bind with c(alpha, g_i, beta, h_i, Initial Beta, error).

Methods

`signature(TS_eSet = "ExpressionSet")` This method is created for the function `row_optimize`.

Author(s)

Yang, X-Y, Dent, Jennifer E. and Nardini, C.

Examples

```
#########Load the SOS pathway data #######
data(sos)

#########Set Slope and Initial Beta #######

Slope<- s_diff(sos)
S<- Slope[1,] #S is the slope of the row you want to calculate. You can either input a vector yourself.
```

```
beta<- runif(n=1,min=1,max=10)

#########Set parameters #######
sparsity<- 0.2
lbH<- -3
ubH<- 3
lbB<- 0
ubB<- 10

#########Calculate results #######

result_r<-row_optimize(sos,S,beta,sparsity,lbH,ubH,lbB,ubB)
```

---

s_diff *Calculate slopes from time points and time series matrix.*

Description

This function allows users calculate slopes from time points and time series data.

Usage

```
## S4 method for signature 'ExpressionSet'
s_diff(TS_eSet)
```

Arguments

TS_eSet	Time series data in ExpressionSet class. assayData: Matrix with n metabolite in row and m time points in column. phenoData: phenoData type. The sample data.frame should include the label "time", which represents the values of time points.

Value

This function directly return a slope matrix.

Methods

`signature(TS_eSet = "ExpressionSet")` This method is created for function `s_diff`.

Author(s)

Yang, X-Y, Dent, Jennifer E. and Nardini, C.

Examples

```
#########Load the SOS pathway data #######
data(sos)

#########Calculate results #######

Slope<-s_diff(sos)
```

---

sos *SOS pathway time series data*

Description

In this package we offer the SOS data obtained from Uri Alon's lab (http://www.weizmann.ac.il/mcb/UriAlon/). SOS response is a general DNA repair system in bacteria which allows survival after DNA damage. This SOS dataset is taken from real experiment expression data in *Escherichia coli*. It contains 8 genes under Experiment 3 (UV light intensities, 4:20 Jm^(-2)).

Usage

```
data(sos)
```

Format

sos.data is time series gene expression value data in ExpressionSet Class. assayData: Matrix with expression values of 8 genes in SOS pathway of *Escherichia coli*. These expression levels are observed at 50 time points. phenoData: Sample data.frame includes label "time", which represents the value of time points.

References

M. Ronen, R. Rosenberg, B. I. Shraiman, and U. Alon. Assigning numbers to the arrows: parameterizing a gene regulation network by using accurate expression kinetics. Proceedings of the National Academy of Sciences of the United States of America, Aug. 2002. PMID: 12145321.

Examples

```
data(sos)
```

SPEM *S-system parameter estimation method*

Description

This function calculates parameters of S-system from entire time series matrix.

Usage

```
## S4 method for signature 'ExpressionSet'
SPEM(TS_eSet, n = 3, sparsity = 0.2, lbH = -3, ubH = 3, lbB = 0, ubB = 10)
```

Arguments

TS_eSet	Time series data in ExpressionSet class. assayData: Matrix with n metabolite in row and m time points in column. phenoData: phenoData type. The sample data.frame should include the label "time", which represents the values of time points.
n	Positive integer, SPEM will guess initial beta n times.
sparsity	A positive number. In order to force the interaction matrix to be sparse, interactions with absolute value smaller than "sparsity" will be set to zero.
lbH	Lower boundary value of h.
ubH	Upper boundary value of h.
lbB	Lower boundary value of beta.
ubB	Upper boundary value of beta.

Details

In this SPEM package, we aim to reconstruct gene networks from time-series expression data using the S-system model. The input dataset should be as an ExpressionSet data container, describing, in assayData, expression data for n genes (rows) and m time points (columns), along with a vector of length m, which records the exact values of time points, thus showing the sample intervals in phenoData. SPEM will calculate the parameters alpha, G, beta and H of the S-system function set that best fits the dataset.

Value

alpha, G, beta, H	Parameters of the reconstructed S-system.
IniBeta	Guess of the IniBeta value (Picked randomly by SPEM itself).
error	Regression error.

Methods

signature(TS_eSet = "ExpressionSet") This method is created for function SPEM.

Author(s)

Yang, X-Y., Dent, Jennifer E. and Nardini, C.

Examples

```
#########Generate Toy Model #######
#########
# If you want to calculate SOS dataset in this package, please read our vignette###
#Real dataset takes a long time to calculate. You may want to try function 'row_optimize' to compute it in parallel##


toy_expression_data<-matrix(data=abs(rnorm(12)),nrow=3,ncol=4, dimnames=list(paste("G",c(1:3),sep=''), paste("t
toy_timepoints_data<-data.frame(index=c(1:4), label=paste("tp",c(0,2,4,6),sep='_'), time=c(0,2,4,6),row.names=p
toy_varMetadata<-data.frame(labelDescription=c("Index number","Label Detail", "Time points values"),row.names=c(
toy_phenoData<-new("AnnotatedDataFrame", data=toy_timepoints_data,varMetadata=toy_varMetadata)
toy_ExpressionSet<-new("ExpressionSet", exprs=toy_expression_data,phenoData=toy_phenoData)

#########Set parameters #######
n<- 1
sparsity<- 0.2
lbH<- -3
ubH<- 3
lbB<- 0
ubB<- 10
#########Calculate results #######

result<-SPEM(toy_ExpressionSet,n,sparsity,lbH,ubH,lbB,ubB)
```

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