Package ‘SPEM’

January 15, 2017

Type Package
Title S-system parameter estimation method
Depends R (>= 2.15.1), Rsolnp, Biobase, methods
Version 1.14.0
Date 2013-1-12
Author Xinyi YANG Developer, Jennifer E. DENT Developer and Christine NARDINI Supervisor
Maintainer Xinyi YANG <yangxinyi@picb.ac.cn>
Description This package can optimize the parameter in S-system models given time series data
License GPL-2
LazyLoad yes
biocViews Network, NetworkInference, Software
NeedsCompilation no

R topics documented:

SPEM-package .......................................................... 1
row_optimize .......................................................... 2
sos ................................................................. 3
SPEM ............................................................... 4
s_diff ............................................................... 6

Index

<table>
<thead>
<tr>
<th>SPEM-package</th>
<th>S-system parameter estimation method package</th>
</tr>
</thead>
</table>

Description

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

Details
row_optimize

## 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.

### 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

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

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


Examples
data(sos)

---

**SPEM**

\(S\)-system parameter estimation method

Description

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

Usage

```r
## 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 para##

toy_expression_data<-matrix(data=abs(rnorm(12)),nrow=3,ncol=4, dimnames=list(paste("G",c(1:3),sep=""), pastet("tp",c(0,2,4,6),sep='_'))

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=paste("tp",c(0,2,4,6),sep='_'))

toy_varMetadata<-data.frame(labelDescription=c("Index number","Label Detail", "Time points values"),row.names=c("index","label","time"))

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

#########Calculate results #######
Slope<-s_diff(sos)
```
Index

*Topic Bioinformatics, NetworkAnalysis, NetworkInference, Software
  SPEM, 4
*Topic Datasets
  sos, 3
*Topic Package
  SPEM-package, 1
*Topic Reconstruction
  row_optimize, 2
*Topic Slope
  s_diff, 6

row_optimize, 2
row_optimize,ExpressionSet-method
  (row_optimize), 2

s_diff, 6
s_diff,ExpressionSet-method(s_diff), 6
sos, 3
SPEM, 4
SPEM,ExpressionSet-method(SPEM), 4
SPEM-package, 1