Package ‘SPEM’

March 29, 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 7

---

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
row_optimize

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

```r
## 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)
```

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 parallel##

toy_expression_data<-matrix(data=abs(rnorm(12)),nrow=3,ncol=4, dimnames=list(paste("G",c(1:3),sep=""), paste("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 to 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 returns 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