

# Package ‘SPEM’

April 25, 2025

**Type** Package

**Title** S-system parameter estimation method

**Depends** R (>= 2.15.1), Rsolnp, Biobase, methods

**Version** 1.49.0

**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

**git\_url** <https://git.bioconductor.org/packages/SPEM>

**git\_branch** devel

**git\_last\_commit** 137e464

**git\_last\_commit\_date** 2025-04-15

**Repository** Bioconductor 3.22

**Date/Publication** 2025-04-24

## Contents

|                        |          |
|------------------------|----------|
| SPEM-package . . . . . | 2        |
| row_optimize . . . . . | 2        |
| sos . . . . .          | 4        |
| SPEM . . . . .         | 4        |
| s_diff . . . . .       | 6        |
| <b>Index</b>           | <b>7</b> |

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[,] #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)
```

---

 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<sup>-2</sup>).

### 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("H",c(1:4),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=c("G1","G2","G3"),
toy_varMetadata<-data.frame(labelDescription=c("Index number","Label Detail", "Time points values"),row.names=c("G1","G2","G3"),
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

```

## 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)

```

# Index

- \* **Bioinformatics, NetworkAnalysis,  
NetworkInference, Software**
  - SPEM, [4](#)
- \* **Datasets**
  - sos, [4](#)
- \* **Package**
  - SPEM-package, [2](#)
- \* **Reconstruction**
  - row\_optimize, [2](#)
- \* **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, [4](#)  
SPEM, [4](#)  
SPEM, ExpressionSet-method (SPEM), [4](#)  
SPEM-package, [2](#)