${\bf Package~'gLVInterNetworks'}$

December 19, 2016

Type Package		
Title Inference of interaction networks based on generalised Lotka Volterra dynamics		
Version 0.1		
Date 2016-11-08		
Author Lukas Hirsch, Florian Centler		
Maintainer Lukas Hirsch < lukashirsch@gmail.com>		
Description Inference of interaction networks based on the parameterization of generalized Lotka Volterra models on timeseries data		
Imports deSolve, MASS, glmnet, FME, igraph, minpack.lm, coda, minqa, rootSolve		
License GPL-2		
R topics documented:		
gLVInterNetworks-package gLVInterNetworks-package generate_data gLVlinearRegression gLVnonlinearRegression plot.Sim_data plotGraph sensitivityAnalysis		
gLVInterNetworks-package Inference of interaction networks based on generalised Lotka Volterra dynamics		

Description

Inference of interaction networks based on the parameterization of generalized Lotka Volterra models on timeseries data

Details

The DESCRIPTION file: This package was not yet installed at build time.

Index: This package was not yet installed at build time. ~~ An overview of how to use the package, including the most important functions ~~

Author(s)

Lukas Hirsch, Florian Centler Maintainer: Lukas Hirsch <lukashirsch@gmail.com>

References

~~ Literature or other references for background information ~~

Examples

```
library(gLVInterNetworks)
data <- generate_data(species = 2, number_of_non_diagonal_coefficients = 2, timepoints = 100, noise = 0.01, t
## Not run: plot(data, type = "l")
lr <- gLVlinearRegression(data, regularization = TRUE, alpha = 0)</pre>
## Not run: summary(lr)
## Not run: plot(lr, type = "1")
## Not run: points(data)
nlr <- nongLVlinearRegression(data, parms0 = lr$Parms)</pre>
## Not run: summary(nlr)
## Not run: plot(nlr, type = "l")
## Not run: points(data)
## Not run: par(mfrow = c(1,2))
## Not run: plotGraph(data, vsize = 0.2, main = "Original interaction network", verbose = TRUE )
## Not run: plotGraph(nlr, vsize = 0.2, main = "Inferred interaction network", verbose = TRUE)
ident <- sensitivityAnalysis(nlr$Parms)</pre>
## Print summary of sensitivity matrix
summary(ident$sens)
## Print collinearity index for all parameters together
ident$coll[ident$coll[,"N"]==length(data$Parms),]
```

gLVInterNetworks-package

Inference of interaction networks based on generalised Lotka Volterra dynamics

Description

Inference of interaction networks based on the parameterization of generalized Lotka Volterra models on timeseries data

Details

The DESCRIPTION file: This package was not yet installed at build time.

Index: This package was not yet installed at build time.

~~ An overview of how to use the package, including the most important functions ~~

generate_data 3

Author(s)

Lukas Hirsch, Florian Centler Maintainer: Lukas Hirsch < lukashirsch@gmail.com>

References

~~ Literature or other references for background information ~~

Examples

```
library(gLVInterNetworks)
data <- generate_data(species = 2, number_of_non_diagonal_coefficients = 2, timepoints = 100, noise = 0.01, t
## Not run: plot(data, type = "l")
lr <- gLVlinearRegression(data, regularization = TRUE, alpha = 0)
## Not run: summary(lr)
## Not run: plot(lr, type = "l")
## Not run: points(data)
nlr <- gLVnonlinearRegression(data, parms0 = lr$Parms)
## Not run: summary(nlr)
## Not run: plot(nlr, type = "l")
## Not run: points(data)
## Not run: points(data)
## Not run: points(data)
## Not run: plotGraph(data, vsize = 0.2, main = "Original interaction network", verbose = TRUE)
## Not run: plotGraph(nlr, vsize = 0.2, main = "Inferred interaction network", verbose = TRUE)</pre>
```

generate_data

Generate random data for gLV fitting

Description

Generates random data simulating time series of cell abundances governed by Lotka Volterra dynamics

Usage

```
generate_data(species, number_of_non_diagonal_coefficients, timepoints, noise, testData)
```

Arguments

species Integer describing the number of independent cellular subcommunities

number_of_non_diagonal_coefficients

Integer describing the number of non-zero interactions present in the simulated system. These are assigned randomly between the nodes or subcommunities

timepoints Numeric vector containing the timepoints for which to compute the solutions of the model

noise The standard deviation of the normally distributed stochastic factor added to the solution of the model at each time step

testData Number of observations used as test dataset for validation on untrained data, taken from the last measurements of the time series.

Value

Returns a matrix. The first column displays the time points, and the remaining columns correspond each to a independent variable in the system.

Author(s)

Lukas Hirsch

Examples

```
##---- Should be DIRECTLY executable !! ----
##-- ==> Define data, use random,
##--or do help(data=index) for the standard data sets.
## The function is currently defined as
function (species, number_of_non_diagonal_coefficients, timepoints,
    noise)
    "requires inSilico_bio, discrete, addNoise_res"
    raw_data <- inSilico_bio(species, number_of_non_diagonal_coefficients)</pre>
    Parms <- raw_data[[2]]</pre>
    res <- raw_data[[1]]</pre>
    threshold = 3
    if (any(which(round(diff(abs(rowMeans(res[, -1])), 2), threshold) ==
        end <- min(which(round(diff(abs(rowMeans(res[, -1])),</pre>
            2), threshold) == 0))
    }
    else {
        end <- nrow(res)</pre>
    }
    res <- solveLV_bio(Parms, seq(0, end, by = 0.01), res[1,
    discretization <- nrow(res)/timepoints</pre>
    res <- discrete(res, discretization)</pre>
    test_data <- res[(nrow(res) - 19):nrow(res), ]</pre>
    obs <- res[1:(nrow(res) - 20), ]
    obs <- addNoise_res(obs, noise)</pre>
    timepoints <- nrow(obs)</pre>
    dimensions <- ncol(obs[, -1])</pre>
    k <- sum(any(Parms == 0))/length(Parms)</pre>
    data <- list(species = species, timepoints = timepoints,</pre>
        Parms = Parms, noise = noise, sparsity = k, obs = obs,
        testData = test_data)
    class(data) <- "Sim_data"</pre>
    return(data)
  }
```

gLVlinearRegression Parameter estimation of algebraic linear discrete gLV model

Description

Given multivariatic time series data, this function fits a linear and discrete generalized Lotka Volterra model of the form $\beta = \alpha + \beta = \alpha +$

gLVnonlinearRegression

Usage

```
gLVlinearRegression(data, regularization = FALSE, alpha = 0)
```

Arguments

data Matrix or table containing time series of measurements in longitudinal form

where first column corresponds to the time points and subsequent columns cor-

5

respond to each model variable

regularization Boolean flag if regularization of the parameter matrix should be forced

alpha Regularization parameter for the elastic net. It ranges from 0 (= Ridge regres-

sion) to 1 (= LASSO regression) with values in between corresponding to both

L1 and L2 penalties weighted by alpha

Details

Some theory and formulas on elastic net

gLVnonlinearRegression

Parameter estimation through gradient search of continuous nonlinear gLV model

Usage

```
gLVnonlinearRegression(data, parms0 = NULL, ftol = 1e-8, ptol = 1e-8, maxiter = 100, lowerbound =
```

Arguments

data	Data input containing a time series of observations in longitudinal matrix form
parms0	Optional. Starting parameter vector. Default = Zero vector
ftol	Objective function output tolerance before stopping iterative optimization
ptol	Parameter change tolerance in output of objective function
maxiter	Maximal number of iterations allowed before breaking the gradient search algorithm
lowerbound	Numerical vector of equal length as parameter vector describing lower bound for constrained parameter search
upperbound	Numerical vector of equal length as parameter vector describing upper bound for constrained parameter search
method	Method used for optimization of the objective function. Default is "Marq" for Leverberg-Marquandt

Examples

```
##--- Should be DIRECTLY executable !! ----
##-- ==> Define data, use random,
##--or do help(data=index) for the standard data sets.
```

6 plotGraph

plot.Sim_data

Plot function for objects returned by in silico data generation function

Usage

```
plot.Sim_data(x, legend = FALSE, ...)
```

Arguments

x Object of class Sim_data as returned by function generate_data() legend Set to TRUE to place a basic legend in the topright of the plot ...

Examples

```
##---- Should be DIRECTLY executable !! ----
##-- ==> Define data, use random,
##--or do help(data=index) for the standard data sets.
## The function is currently defined as
function (x, ...)
{
    matplot(x$obs[, -1])
}
```

plotGraph

Plot interaction network

Description

Plots a graph representing the interaction network described by the data

Usage

```
plotGraph(x, vsize = 0.1, main = NULL, verbose = FALSE, keepNames = FALSE, ...)
```

Arguments

x Object containing parameter matrix in form of x\$Parmsvsize Integer inversely proportional to the size of the nodes

main Title of the plot

verbose Include edge values in output network

keepNames Set to TRUE if plotted Network should keep the names of the variables as given

in the observations table. Default = FALSE

. . .

Value

igraph object

sensitivityAnalysis 7

Author(s)

Lukas Hirsch

Examples

```
data <- generate_data(2,2,100,0.1, 20)
#plotGraph(data)
##---- Should be DIRECTLY executable !! ----
##-- ==> Define data, use random,
##--or do help(data=index) for the standard data sets.
```

sensitivityAnalysis

Compute parameter correlations and multicollinearity for the model output

Description

This function is a wrapper function for sensFun and Collin from package FME. It calculates both a sensitivity matrix S_ij and multicollinearity index for all parameter combinations.

Usage

```
sensitivityAnalysis(Parms)
```

Arguments

Parms

Numeric vector or matrix with the parameter coefficients to test

Value

List containing:

sens Matrix containing sensitivity output values for each parameter and each model

variable. The sensitivity matrix S_ij contains elements dy_i/dpar_j*parscale_j/varscale_i.

The scale used to change the value of each parameter can be seen using the summary function on the sens table, and it is set to be the same value of the parameter

itself

coll Table with collinearity index for each possible parameter subset.

Warning

The function needs the original data as a global variable called "data". Please make sure that when using this function to perform identifiability analysis on a set of parameters, that the observation matrix or table used to estimate the parameter set is accessible under the name "data"

Note

For details in output interpretation see package FME

Index

```
*Topic \textasciitildekwd1
    generate_data, 3
*Topic \textasciitildekwd2
    generate_data, 3
    gLVlinearRegression, 4
    {\tt gLVnonlinearRegression}, {\tt 5}
    plotGraph, 6
    sensitivity Analysis, 7
*Topic package
    gLVInterNetworks-package, 1, 2
{\tt generate\_data}, {\tt 3}
{\tt gLVInterNetworks}
         (gLVInterNetworks-package), 1, 2
gLVInterNetworks-package, 1, 2
gLVlinearRegression, 4
{\tt gLVnonlinearRegression}, {\tt 5}
plot.Sim_data, 6
plotGraph, 6
{\tt sensitivityAnalysis}, {\tt 7}
```