Package ‘CellNOptR’

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Type Package

Title Training of boolean logic models of signalling networks using prior knowledge networks and perturbation data.

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Suggests RUnit, BiocGenerics, igraph

biocViews CellBasedAssays, CellBiology, Proteomics, TimeCourse

Description

This package does optimisation of boolean logic networks of signalling pathways based on a previous knowledge network and a set of data upon perturbation of the nodes in the network.

License GPL-3

LazyLoad yes

SystemRequirements Graphviz version >= 2.2

NeedsCompilation yes

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**Description**

This package does optimisation of boolean logic networks of signalling pathways based on a previous knowledge network and a set of data collected upon perturbation of some of the nodes in the network.

**Details**

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**Author(s)**

T. Cokelaer, A. MacNamara, F. Eduati, S. Schrier, C. Terfve

Maintainer: T. Cokelaer <cokelaer@ebi.ac.uk>

**References**


**Examples**

```r
library(CellNOptR)

# quick 1 time point optimisation of a Prior Knowledge Network to MIDAS data.
data(CNOlistToy, package="CellNOptR")
data(ToyModel, package="CellNOptR")

pknmodel = ToyModel
cnolist = CNOlist(CNOlistToy)
model = preprocessing(cnolist, pknmodel)
results = gaBinaryT1(cnolist, model, verbose=FALSE)
plotFit(results)
cutAndPlot(cnolist, model, list(results$bString))

# Same as above and HTML report
```
checkSignals

CNORwrap(name="Toy",
         namesData=list(CNOlist="ToyData",model="ToyModel"),
         data=CNOlistToy, model=pknmodel)

checkSignals  Check the CNOlist and model matching

Description

This function checks that all the signals in a CNOlist match to species in the model. It also checks
that the CNOlist and Model lists have the right format and contain the right fields. It is called by the
preprocessing function so there is no need to call it directly anymore if you use the preprocessing
function.

In version 1.3.20, check of inhibitors and stimuli is also performed.

Usage

checkSignals(CNOlist, model)

Arguments

  CNOlist  A CNOlist structure, as created by makeCNOlist.
  model    A model structure, as created by readSIF.

Details

If the formats are wrong, this function produces an error. If the signals/inhibitors/stimuli do not
match the species, this function produces a warning that explains which signals does no match any
species.

Author(s)

  C. Terfve, T. Cokelaer

See Also

  makeCNOlist, readSIF, preprocessing

Examples

data(CNOlistToy, package="CellNOptR")
data(ToyModel, package="CellNOptR")
checkSignals(CNOlistToy, ToyModel)
CNOdata

Get data from a CellNOpt data repository

Description

This function fetch a file from the URL provided (default is http://www.ebi.ac.uk/~cokelaer/cellnopt/data/_downloads) and save it into a temporary file.

You will need Rcurl package to use this function.

Usage

CNOdata(filename, verbose=FALSE, url=NULL)

Arguments

filename
   a valid filename that can be found in the url

verbose
   FALSE by default, it prints the path of the temporary file where data has been copied.

url
   You can overwrite the default URL (http://www.ebi.ac.uk/~cokelaer/cellnopt/data/_downloads) with this argument.

Value

the path of the temporary file where data has been copied.

Author(s)

T. Cokelaer

Examples

readSIF(CNOdata("PKN-ToyMMB.sif"))

CNOlist-class

Class "CNOlist"

Description

This function takes as input the filename of a MIDAS file (or the list returned by makeCNOlist) and returns an instance of CNOlist class. It provides an object oriented approach to manipulate CNOlist. This function calls readMIDAS and makeCNOlist.

Objects from the Class

Objects can be created by calls of the form new("CNOlist", ...).
Slots

cues: Object of class "matrix"
ihibitors: Object of class "matrix"
stimuli: Object of class "matrix"
signals: Object of class "list"
variances: Object of class "list"
timepoints: Object of class "vector" timepoints contained in the signals matrix.

See CNOlist-methods for details.

Methods

Available methods are plot, compatCNOlist, randomize, length. See CNOlist-methods for details.

Author(s)

T. Cokelaer

See Also

randomizeCNOlist, plotCNOlist, plotCNOlist2

Examples

showClass("CNOlist")

files<-dir(system.file("ToyModel",package="CellNOptR"),full=TRUE)
cnolist = CNOlist(files[[1]])
#
getters:
getCues(cnolist)
getInhibitors(cnolist)
getSignals(cnolist)
getVariances(cnolist)
getTimepoints(cnolist)
getStimuli(cnolist)
#
In version 1.3.30 and above, use the plot method instead of former plotCNOlist function.
plot(cnolist)
new_cnolist = randomize(cnolist)
length(cnolist)

CNOlist-methods

List of CNOlist-class methods

Description

CNOlist is a class with a set of methods described here below.

Usage

signature(x="CNOlist")
Getters

getCues  Returns the cues (matrix) found in the CNOlist
getSignals Returns the signals (list of matrices) found in the CNOlist
getStimuli Returns the cues found in the CNOlist
getInhibitors Returns the inhibitors found in the CNOlist
getTimepoints Returns the timepoints found in the CNOlist
getVariance Returns the Variances (list of matrices) found in the CNOlist. Will be different from zero only if replicates were found in the MIDAS data. See makeCNOlist

Setters

setSignals Set the signals. No sanity check!

Other methods

compatCNOlist convert the instance CNOlist into the old-style returned by makeCNOlist that is a list. Used in the ODE package.
length returns length of CNOlist (number of time points)
randomize randomizes the signals matrice in a CNOlist. See randomizeCNOlist for details
show prints summary information
plot plot the CNOlist instance using the plotCNOlist function.
plot signature(x="CNOlist", y="CNOlist"): Please see the page of plotCNOlist2 for more details.

Author(s)

T.Cokelaer

See Also

CNOlist-class, randomizeCNOlist makeCNOlist

Examples

showClass("CNOlist")
data(CNOlistToyMMB, package="CellNOptR")
cnolist = CNOlistToyMMB

# In version 1.3.30 and above, use the plot method instead of former plotCNOlist function.
plot(cnolist)

# In version 1.5.14 and above, use getters instead of the @ operator
getCues(cnolist)

# others:
new_cnolist = randomize(cnolist)
**CNOlistDREAM**  
*Data used for the DREAM3 challenge*

**Description**

This data object contains the DREAM data used in the package vignette, already loaded and formatted as a CNOlist object. This is to be used with the model "DreamModel". This is a data collected on HepG2 cells cultivated with or without stimulation of tgfα, ilk, mek12, pi3k and p38, in combination with inhibition of igf1 and/or il1a. Seven phosphoproteins are measured using Luminex xMAP assays: akt, erk12, ikb, jnk12, p38, hsp27 and mek12.

**Usage**

CNOlistDREAM

**Format**

CNOlistDREAM is a list with the fields "namesCues" (character vector), "namesStimuli" (character vector), "namesInhibitors" (character vector), "namesSignals" (character vector), "timeSignals" (numerical vector), "valueCues" (numerical matrix), "valueInhibitors" (numerical matrix), "valueStimuli"(numerical matrix), "valueSignals"(numerical matrix).

**Source**

This data and model is extracted from the Matlab version of CellNOpt1.0 ([http://www.ebi.ac.uk/saezrodriguez/software.html#CellNetOptimizer](http://www.ebi.ac.uk/saezrodriguez/software.html#CellNetOptimizer)).

**References**


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**CNOlistToy**  
*Toy data*

**Description**

This data object contains the data associated with the Toy Model example from the package vignette, already loaded and formatted as a CNOlist object.

**Usage**

CNOlistToy
Format

CNOlistToy is a list with the fields "namesCues" (character vector), "namesStimuli" (character vector), "namesInhibitors" (character vector), "namesSignals" (character vector), "timeSignals" (numerical vector), "valueCues" (numerical matrix), "valueInhibitors" (numerical matrix), "valueStimuli" (numerical matrix), "valueSignals" (numerical matrix).

Source

This data and model is extracted from the Matlab version of CellNOpt1.0 (http://www.ebi.ac.uk/saezrodriguez/software.html#CellNetOptimizer).

References

CNORbool  

Simple Boolean analysis standalone

Description

This function performs the optimisation of a PKN model to a CNOlist data set. It optimises each time point found in the data and returns the processed model as well as a list of optimised bitstring corresponding to each time points that has been optimised.

This function does not create any plots or reports unlike CNORwrap.

Usage

CNORbool(CNOlist, model, paramsList=defaultParameters(),
  compression=TRUE, expansion=TRUE, cutNONC=TRUE, verbose=FALSE,
  timeIndices = NULL)

Arguments

- **CNOlist**
  a CNOlist structure, as created by makeCNOlist or a MIDAS filename
- **model**
  a model structure, as created by readSIF or a SIF filename.
- **paramsList**
  Parameters of the genetic algorithm. If not provided, it is populated with the defaultParameters function.
- **compression**
  compress the model (default TRUE)
- **expansion**
  expand the gates (default TRUE)
- **cutNONC**
  cut the NONC nodes off the model by (default TRUE)
- **verbose**
  FALSE
- **timeIndices**
  by default, optimise T1 and T2 assuming there are the 2 first time points. However, with this argument you can change that behaviour to arbitrary time points.

Value

This function returns 2 components. The first one is the processed model used in the optimisation. The second is a list of optimised bitstrings found for each time points available in the MIDAS data set.

Author(s)

T.Cokelaer, S.Schrier

Examples

data(CNOlistToy,package="CellNOptR")
data(ToyModel,package="CellNOptR")
res = CNORbool(CNOlist=CNOlistToy, model=ToyModel)
CNORwrap

Description

This function is a wrapper around the whole CNOR analysis, it performs the following steps:

1. Plot the CNOlist;
2. Checks data to model compatibility;
3. Call the preprocessing function (Cut the nonC off the model, compress the model and expand the gates);
4. Compute the residual error;
5. Prepare for simulation;
6. Optimisation T1 and T2 (optional);
7. Plot simulated and experimental results;
8. Plot the evolution of fit;
9. Write the scaffold and PKN;
10. Write the report

Usage

CNORwrap(paramsList=NA, data=NA, model=NA, name, namesData=NA, time=1, compression=TRUE, expansion=TRUE, cutNONC=TRUE)

Arguments

paramsList A list of parameters related to the Genetic Algorithm parameters:
1. sizeFac: default to 1e-04;
2. NAFac: default to 1; popSize: default to 50;
3. pMutation: default to 0.5;
4. maxTime: default to 60;
5. maxGens: default to 500;
6. stallGenMax: default to 100;
7. selPress: default to 1.2;
8. elitism: default to 5;
9. relTol: default to 0.1;
10. verbose: default to FALSE (default to true in the functions used by CNORwrap but CNORwrap sets them to false by default).

and the Data and Model structure.
If paramsList is not provided (NA), it is filled internally with the defaultParameters function.
If Data and Model are not provided in paramsList, the function looks for Data and Model arguments.
If Data and Model are provided, the function overwrites the field data and model in paramsList.

data a CNOlist structure, as created by makeCNOlist
model a model structure, as created by readSIF.
name a string that will be used to name the project and all graphs produced
namesData a list with two elements: CNOlist and Model, each containing a string that is a reference for the user to know which model/data set was used (it will be included in the report). If not provided, the list is built automatically using the name arguments.
time either 1 or 2: Do you want to perform a one time point steady state optimisation or a 2 time points pseudo steady state optimisation. By default this is set to 1.
compression compress the model (default TRUE)
expansion expand the gates (default TRUE)
cutNONC cut the NONC nodes off the model by (default TRUE)

details
If you do not provide a parameters list, you can provide only essential elements, and all other parameters will be set to their default values. In this case, you should set paramsList=NA, and provide the following fields: data, model, name, time.

value
This function does not return anything, it does the analysis, produces all the plots and puts them in a folder that is in your working directory, and is called "Name".

author(s)
C. Terfve

examples
#version with paramslist
tmpdir<-tempdir()
setwd(tmpdir)
data(CNOlistToy,package="CellNOptR")
data(ToyModel,package="CellNOptR")

plist = defaultParameters(CNOlistToy, ToyModel)
plist$maxGens = 5
plist$popSize = 5

CNORwrap(paramsList=plist, name="Toy",
    namesData=list(CNOlist="ToyData", model="ToyModel"))

## Not run:
#version with default parameters
data(CNOlistToy,package="CellNOptR")
data(ToyModel,package="CellNOptR")

CNORwrap(name="Toy",
    namesData=list(CNOlist="ToyData",model="ToyModel"),
data=CNOlistToy, model=ToyModel)
compressModel

Compress a model

Description

This function compresses a model by compressing species that are not signals/inhibited/stimulated and that are not dead ends/in complex logic (i.e. only species with either one input or one output are compressed)/in self loops.

You can also use preprocessing function instead that calls compressModel and other preprocessing functions.

Usage

compressModel(model, indexes)

Arguments

- model: a model structure as produced by readSIF.
- indexes: list of indexes of the species stimulated/inhibited/measured in the model, as created by indexFinder.

Details

Be aware that in the multiple inputs/one output case, if one of the outputs is an `&` gate this function handles it fine as long as it is an `&` with 2 inputs and no more.

Value

a compressed model list, with an additional field called 'speciesCompressed' that contains the names of the species that have been compressed

Note

No need to call this function directly since version 0.99.24. Use preprocessing instead.

Author(s)

C. Terfve

See Also

indexFinder, readSIF, preprocessing

Examples

#load data
data(CNOlistToy,package="CellNOptR")
data(ToyModel,package="CellNOptR")
indicesToy<-indexFinder(CNOlistToy,ToyModel,verbose=FALSE)
toyComp<-compressModel(ToyModel,indicesToy)
computeScoreT1

Compute the score of a model/data set using a bitString to cut the model.

Description

The bitString made of 0 and 1 allows to select a submodel from the model provided. Then, the simulator function are called to compute the objective function. The sizeFac and NAFac are penalties added to the final score as described in gaBinaryT1. The indexList and simList arguments can be provided to speed up the code otherwise, they are recomputed from the CNOlist and model.

Usage

computeScoreT1(CNOlist, model, bString, simList=NULL, indexList=NULL, sizeFac=0.0001, NAFac=1, timeIndex=2)

Arguments

- **CNOlist**: a CNOlist structure, as created by makeCNOlist.
- **model**: a model structure, as created by codereadSIF, normally pre-processed but that is not a requirement of this function.
- **bString**: a bitstring of the same size as the number of reactions in the model above
- **simList**: If provided, simList should be created by prep4sim, that has also already been cut to contain only the reactions to be evaluated.
- **indexList**: If provided, indexList should contain a list of indexes of the species stimulated/inhibited/measured in the model, as created by indexFinder.
- **sizeFac**: the scaling factor for the size term in the objective function, default to 0.0001
- **NAFac**: the scaling factor for the NA term in the objective function, default to 1
- **timeIndex**: the index of the time point to optimize. Must be greater or equal to 2 (1 corresponds to time=0). Must be less than the number of time points. Default is 2.

Value

-score: See gaBinaryT1 for details

Author(s)

T. Cokelaer

Examples

data(CNOlistToy, package="CellNOptR")
data(ToyModel, package="CellNOptR")
model <- preprocessing(CNOlistToy, ToyModel)
score = computeScoreT1(CNOlist(CNOlistToy), model, bString=rep(1,16))
**computeScoreTN**

*Compute the score at TN of a model/data set using a bitString to cut the model.*

**Description**

The bitString made of 0 and 1 allows to select a submodel from the model provided. Then, the simulator function are called to compute the objective function. The sizeFac and NAFac are penalties added to the final score as described in `gaBinaryTN`.

**Usage**

```r
computeScoreTN(CNOlist, model, simList=NULL, indexList=NULL, simResPrev=NULL, bStringPrev=NULL, bStringNext=NULL, timeIndex=NULL, sizeFac=0.0001, NAFac=1, bStrings=NULL)
```

**Arguments**

- **CNOlist**: a CNOlist structure, as created by `makeCNOlist`.
- **model**: a model structure, as created by `codereadSIF`, normally pre-processed but that is not a requirement of this function.
- **simList**: a simList as created by `prep4sim`, that has also already been cut to contain only the reactions to be evaluated. If not provided, it is recomputed automatically.
- **indexList**: a list of indexes of the species stimulated/inhibited/measured in the model, as created by `indexFinder`. If not provided, it is recomputed automatically.
- **simResPrev**: Results of Previous simulation at time TN-1 step.
- **bStringPrev**: the best bitString at time TN-1.
- **bStringNext**: the bitString to use to compute the score at time TN.
- **timeIndex**: Future feature will allows timeIndex to provide the exact list of indices to cut and plot. For now, it is based on the bitStrings provided.
- **sizeFac**: the scaling factor for the size term in the objective function, default to 0.0001.
- **NAFac**: the scaling factor for the NA term in the objective function, default to 1.
- **bStrings**: list of optimised bitstrings found at the previous time points.

**Value**

- **score**: See `gaBinaryTN` for details.

**Author(s)**

T. Cokelaer, S.Schrier

**Examples**

```r
data(CNOlistToy2, package="CellNOptR")
data(ToyModel2, package="CellNOptR")
model <- preprocessing(CNOlistToy2, ToyModel2)
bStringT1 = c(0,0,1,1,1,1,1,1,0,0,1,1,1,1,1,1)
simT1<-simulateTN(CNOlist=CNOlistToy2, model=model, bStrings=list(bStringT1))
score1 = computeScoreTN(CNOlistToy2, model, bStrings=list(bStringT1,c(1,0,1,0)))
```
cutAndPlot

Interface to cutAndPlotResults functions.

Description

This function takes a model and cnolist as well as a list of optimised bitstring at different time points. It calls the appropriate cutAndPlotResultsTX function.

Usage

cutAndPlot(CN0list, model, bStrings, plotPDF=FALSE, tag=NULL, plotParams = list(maxrow = 10))

Arguments

CN0list a CN0list, corresponding to the optimisation one
model a model (the full one that was used for optimisation)
bStrings a bitstring for T1 as output by gaBinaryT1 (i.e. a vector of 1s and 0s)
plotPDF TRUE or FALSE; tells whether you want a pdf to be produced or not
tag NULL or string; tells whether you want to prefix filenames with a tag (replaces the default behaviour).
plotParams a list of option related to the PDF and plotting outputs. (1) maxrow is the maximum number of row used to plot the results. See plotOptimResultsPan for other fields.

Value

This function returns nothing. It plots a graph in your graphic window and save it in a file if asked

Author(s)

T. Cokelaer

See Also

cutAndPlotResultsT1

Examples

#load data

data(CN0listToy, package="CellNOptR")
data(ToyModel, package="CellNOptR")

#pre-process model
model = preprocessing(CN0listToy, ToyModel)

cutAndPlot(CN0listToy, model, 
bStrings=list(rep(1,length(model$reacID))),plotPDF=FALSE)
**cutAndPlotResultsT1**  
*Plot the results of an optimisation at t1*

**Description**

This function takes a model and an optimised bitstring, it cuts the model according to the bitstring and plots the results of the simulation along with the experimental data.

**Usage**

```r
cutAndPlotResultsT1(model, bString, simList=NULL, CNOlist, indexList=NULL, plotPDF = FALSE, tag = NULL, tPt=CNOlist@timepoints[2], plotParams = list(maxrow=10))
```

**Arguments**

- `model`: a model (the full one that was used for optimisation)
- `bString`: a bitstring for T1 as output by gaBinaryT1 (i.e. a vector of 1s and 0s)
- `simList`: deprecated argument kept for back compatibility. a simlist corresponding to the model, as output by prep4sim
- `CNOlist`: a CNOlist, corresponding to the optimisation one
- `indexList`: deprecated argument kept for back compatibility. an indexList, produced by indexFinder ran on the model and the CNOlist above
- `plotPDF`: TRUE or FALSE; tells whether you want a pdf to be produced or not
- `tag`: NULL or string; tells whether you want to prefix filenames with a tag (replaces the default behaviour).
- `tPt`: The number of time points in the data.
- `plotParams`: a list of option related to the PDF and plotting outputs. (1) maxrow is the maximum number of row used to plot the results. See `plotOptimResultsPan` for other fields.

**Value**

This function returns plotted MSEs and list of filenames generated (if any)

**Author(s)**

C.Terfve, T. Cokelaer, A. MacNamara

**See Also**

- `gaBinaryT1`
#load data

data(CNOlistToy, package="CellNOptR")
data(ToyModel, package="CellNOptR")

#pre-process model
model = preprocessing(CNOlistToy, ToyModel)

#optimise
ToyT1opt<-gaBinaryT1(
  CNOlist=CNOlistToy,
  model=model,
  maxGens=20,
  popSize = 10,
  verbose=FALSE)

#plotting

#cutAndPlotResultsT1(model=model,
#CNOlist=CNOlistToy,
#bString=ToyT1opt$bString,
#plotPDF=FALSE)

cutAndPlotResultsTN CNOlistToy, model, bStrings, plotPDF = FALSE, tag=NULL,
plotParams = list(maxrow = 10))

cutAndPlotResultsTN  Plot the results of an optimisation at tN

Description

This function takes a model and an optimised bitstring, it cuts the model according to the bitstring
and plots the results of the simulation along with the experimental data. This function is designed
to work on results of a 2 step optimisation.

Usage

cutAndPlotResultsTN(CNOlist, model, bStrings, plotPDF = FALSE, tag=NULL,
plotParams = list(maxrow = 10))

Arguments

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>CNOlist</td>
<td>a CNOlist, corresponding to the optimisation one</td>
</tr>
<tr>
<td>model</td>
<td>a model (the full one that was used for optimisation)</td>
</tr>
<tr>
<td>bStrings</td>
<td>a list of bitstring at different time points</td>
</tr>
<tr>
<td>plotPDF</td>
<td>TRUE or FALSE, tells whether you want a pdf to be produced or not</td>
</tr>
<tr>
<td>tag</td>
<td>NULL or string; tells whether you want to prefix filenames with a tag (replaces the default behaviour).</td>
</tr>
<tr>
<td>maxrow</td>
<td>maximum number of row in the plot.</td>
</tr>
<tr>
<td>plotParams</td>
<td>a list of option related to the PDF and plotting outputs. (1) maxrow is the maximum number of row used to plot the results. See plotOptimResultsPan for other fields.</td>
</tr>
</tbody>
</table>
cutCNOlist

Value
This function returns plotted MSEs

Note
New in version 1.3.28

Author(s)
T. Cokelaer, A. MacNamara, Sarah Schrier, C. Terfve based on cutAndPlotResultsT1

See Also
gaBinaryT1, prep4sim, cutAndPlotResultsT1

Examples
#load data
data(CNOlistToy2,package="CellNOptR")
data(ToyModel2,package="CellNOptR")

#pre-process model
model = preprocessing(CNOlistToy2, ToyModel2)

#optimise t1
ToyT1<-gaBinaryT1(
    CNOlist=CNOlistToy2,
    model=model,
    maxGens=20,
    popSize = 10,
    verbose=FALSE)

#Optimise T2
ToyT2<-gaBinaryTN(
    CNOlist=CNOlistToy2,
    model=model,
    bStrings=list(ToyT1$bString),
    maxGens=20,
    popSize = 10,
    verbose=FALSE)

cutAndPlotResultsTN(
    CNOlist=CNOlistToy2,
    model=model,
    bStrings=list(ToyT1$bString, bStringT2=ToyT2$bString),
    plotPDF=FALSE)
**cutModel**

**Description**

The MIDAS file may contain species that are not contained in the model. If you want to remove cues and signals from your CNOlist that are not contained in the model, you can use this function by using the parameter model. It can also be used to remove some time points by using the parameter cutTimeIndices. Both parameters can be used at the same time and at least one of them must be provided.

**Usage**

```r
cutCNOlist(cnolist, model, cutTimeIndices, verbose=FALSE)
```

**Arguments**

- `cnolist` the CNOlist structure
- `model` the model
- `cutTimeIndices` the time indices to remove
- `verbose` Set it to True to get the signals and cues not found in the model

**Value**

- `cutCNOlist` the new CNOlist object

**Note**

added in version 1.5.10

**Author(s)**

T. Cokelaer

**See Also**

- CNOlist-class

---

**cutModel**

_Cut a model structure according to a bitstring_

**Description**

This function is for developers only.

**Usage**

```r
cutModel(model, bString)
```

**Arguments**

- `model` the model object to cut.
- `bString` the bitString to be used to cut the model object.
**cutNONC**

**Value**

`cutModel` the new model object

**Note**

added in version 1.3.16

**Author(s)**

T. Cokelaer

---

`cutNONC`  
*Cuts the non-observable/non-controllable species from the model*

**Description**

This function cuts the non-observable and/or non-controllable species from the model, and returns a cut model.

**Usage**

`cutNONC(model, NONCindexes)`

**Arguments**

- `model` a model structure, as produced by readSIF
- `NONCindexes` a vector of indices of species to remove in that model, as produced for example by findNONC

**Details**

This function takes in a model and a vector of indices of species to remove in that model and it removes those species and any reaction involving them (be aware, if you have x&y=z and x is to be removed, then the function produces y=z, because it works by removing entire rows of the model matrices and then removes the columns that do not have either an input or an output). This function could actually be used to cut any species, not only NONC species.

**Value**

a model

**Note**

No need to call this function directly since version 0.99.24. Use preprocessing instead.

**Author(s)**

C. Terfve

**See Also**

`findNONC, readSIF`
**Examples**

```r
data(CNOlistToy, package="CellNOptR")
data(ToyModel, package="CellNOptR")
indicesToy<-indexFinder(CNOlistToy, ToyModel, verbose=FALSE)
ToyNCNONCindices<-findNONC(ToyModel, indicesToy, verbose=FALSE)
ToyNCNONCcut<-cutNONC(ToyModel, ToyNCNONCindices)
```

**cutSimList**  
*Cut a simList structure according to a bitstring*

**Description**

This function is for developers only.

**Usage**

```r
cutSimList(simList, bString)
```

**Arguments**

- `simList`  
  the simList object to cut.
- `bString`  
  the bitString to be used to cut the simList object.

**Value**

- `cutSimList`  
  the new simList object

**Author(s)**

T. Cokelaer

---

**defaultParameters**  
*Create a list of default parameters*

**Description**

This function provides a list of default parameters including the Genetic Algorithm parameters.

**Usage**

```r
defaultParameters(data=NA, model=NA)
```

**Arguments**

- `data`  
  a CNOlist structure, as created by makeCNOlist
- `model`  
  a model structure, as created by readSif, normally pre-processed but that is not a requirement of this function
Details

The list contains the Genetic Algorithm parameter, a verbose option and can be used to store the Data and Model.

Value

params a list with the fields: data, model, verbose and all default parameters of gaBinaryT1

Author(s)

T. Cokelaer

Examples

data(ToyModel, package="CellNOptR")
data(CNOlistToy, package="CellNOptR")
params = defaultParameters(CNOlistToy, ToyModel)

exhaustive

Exhaustive search over the optimisation of a PKN model on MIDAS data.

Description

This function performs an exhaustive search of the parameter space trying all the solutions. It is used internally by the genetic algorithm when a small model has to be optimised and the number of solutions to try is smaller than the number of iterations that the Genetic Algorithm will perform.

Usage

exhaustive(CNOlist, model, shuffle=FALSE, Nmax=NULL, verbose=TRUE, sizeFac = 0.0001, NAFac = 1, relTol=0.1, timeIndex=2)

Arguments

CNOlist a CNOlist on which the score is based (based on valueSignals[[2]], i.e. data at time 1)
model a model structure, as created by readSIF, normally pre-processed but that is not a requirement of this function
shuffle The list of bitstrings is set up arbitrarily. You may want to shuffle it.
Nmax The total number of computation will be 2 to the power N, where N is the size of the model (ReacID field). The total number of computation can be large. You may want to set a maximum number of computation using Nmax.
sizeFac the scaling factor for the size term in the objective function, default to 0.0001
NAFac the scaling factor for the NA term in the objective function, default to 1
relTol the relative tolerance for the best bitstring reported by the genetic algorithm, i.e., how different from the best solution, default set to 0.1 Not yet implemented.
verbose logical (default to TRUE) do you want the statistics of each generation to be printed on the screen?
**expandGates**

*Description*

This function takes in a model and splits all AND gates into ORs. In addition, wherever there are more than one, it creates all possible ANDs combinations of them, but considering only ANDs with 2, 3 or 4 inputs according to the user argument (default is 2).

**Value**

This function returns a list with elements:

- `bString`: the best bitstring
- `bScore`: the best score
- `all_scores`: all scores that have been computed
- `results`: a matrix with columns "Generation","Best_score","Best_bitString","Stall_Generation","Avg_Score_Gen","Best_score_Gen","Best_bit_Gen","Iter_time"
- `stringsTol`: the bitstrings whose scores are within the tolerance
- `stringsTolScores`: the scores of the above-mentioned strings

Note that the field `results` is not yet populated but maybe in the future.

**Author(s)**

T. Cokelaer

**See Also**

`gaBinaryT1`

**Examples**

```r
data(CNOlistToy, package="CellNOptR")
data(ToyModel, package="CellNOptR")

# pre-process model

model = preprocessing(CNOlistToy, ToyModel)

# optimise

results <- exhaustive(
  CNOlist=CNOlistToy,
  model=model,
  shuffle=TRUE,
  Nmax=1000,
  verbose=FALSE)
```

**Description**

This function takes in a model and splits all AND gates into ORs. In addition, wherever there are more than one, it creates all possible ANDs combinations of them, but considering only ANDs with 2, 3 or 4 inputs according to the user argument (default is 2).

**Value**

This function returns a list with elements:

- `bString`: the best bitstring
- `bScore`: the best score
- `all_scores`: all scores that have been computed
- `results`: a matrix with columns "Generation","Best_score","Best_bitString","Stall_Generation","Avg_Score_Gen","Best_score_Gen","Best_bit_Gen","Iter_time"
- `stringsTol`: the bitstrings whose scores are within the tolerance
- `stringsTolScores`: the scores of the above-mentioned strings

Note that the field `results` is not yet populated but maybe in the future.

**Author(s)**

T. Cokelaer

**See Also**

`gaBinaryT1`

**Examples**

```r
data(CNOlistToy, package="CellNOptR")
data(ToyModel, package="CellNOptR")

# pre-process model

model = preprocessing(CNOlistToy, ToyModel)

# optimise

results <- exhaustive(
  CNOlist=CNOlistToy,
  model=model,
  shuffle=TRUE,
  Nmax=1000,
  verbose=FALSE)
```
expandGates

Usage

expandGates(model, ignoreList=NA, maxInputsPerGate=2)

Arguments

model a model structure
ignoreList a list of reactions indices to ignore
maxInputsPerGate maximum number of input per gates (Default is 2; up to 4)

Details

This function returns a model with additional fields that help keep track of the processing done on
the network. I would advice not to overwrite on the initial model but rather to assign the result of
this function to a variable with a different name.

Value

returns a model, with additional fields:

SplitANDs list that contains a named element for each AND reac that has been split, and
each element contains a vector with the names of the of the reactions that result
from the split if nothing was split, this element has the default value $ initialReac
[1] "split1" "split2"

newANDs list that contains an element for each new '&' gate, named by the name of this
new and reac, and containing a vector of the names of the reactions from which
it was created (contains all the reacs in that pool, not the particular ones, this
could be improved)

Note

No need to call this function directly since version 0.99.24. Use preprocessing instead.

Author(s)

C.Terfve. T. Cokelaer, A.MacNamara, Martin-Franz-Xaver Pirkl

Examples

#load data
data(CNOlistToy,package="CellNOptR")
data(ToyModel,package="CellNOptR")

#pre-process the model

indicesToy<-indexFinder(CNOlistToy,ToyModel,verbose=TRUE)
ToyNCNOindices<-findNONC(ToyModel,indicesToy,verbose=TRUE)
ToyNCNOcut<-cutNONC(ToyModel,ToyNCNOindices)
indicesToyNCNOcut<-indexFinder(CNOlistToy,ToyNCNOcut)
ToyNCNOcutComp<-compressModel(ToyNCNOcut,indicesToyNCNOcut)
indicesToyNCNOcutComp<-indexFinder(CNOlistToy,ToyNCNOcutComp)
ToyNCNOcutCompExp<-expandGates(ToyNCNOcutComp, maxInputsPerGate=4)
findNONC

Find the indexes of the non-observable and non controllable species

Description

This function finds the indexes of the non-observable and non controllable species and returns the indices, in the model, of the species to remove

Usage

findNONC(model, indexes, verbose=FALSE)

Arguments

model a model structure, as created by readSIF
indexes a list of indexes of the species stimulated/inhibited/measured, as created by indexFinder from a model.
verbose verbose option (default to FALSE)

Details

This function uses the function floyd.warshall.all.pairs.sp from the package RBGL. Non observable nodes are those that do not have a path to any measured species in the model, whereas non controllable nodes are those that do not receive any information from a species that is perturbed in the data.

Value

a vector of indices of species to remove

Note

No need to call this function directly since version 0.99.24. Use preprocessing instead.

Author(s)

C. Terfve

See Also

cutNONC, indexFinder, readSIF

Examples

data(CNOlistToy, package="CellNOptR")
data(ToyModel, package="CellNOptR")
checkSignals(CNOlistToy, ToyModel)
indicesToy <- indexFinder(CNOlistToy, ToyModel)
ToyNCNOindices <- findNONC(ToyModel, indicesToy)
**gaBinaryT1**

*Genetic algorithm used to optimise a model*

**Description**

This function is the genetic algorithm to be used to optimise a model by fitting to data containing one time point.

**Usage**

```r
gaBinaryT1(CNOlist, model, initBstring=NULL, sizeFac = 1e-04, NAFac = 1, popSize = 50, pMutation = 0.5, maxTime = 60, maxGens = 500, stallGenMax = 100, selPress = 1.2, elitism = 5, relTol = 0.1, verbose=TRUE, priorBitString=NULL, timeIndex=2)
```

**Arguments**

- `CNOlist`: a CNOlist on which the score is based (based on valueSignals[[2]], i.e. data at time 1)
- `model`: a model structure, as created by `readSIF`, normally pre-processed but that is not a requirement of this function
- `initBstring`: an initial bitstring to be tested, should be of the same size as the number of reactions in the model above (model$reacID). Default is all ones.
- `sizeFac`: the scaling factor for the size term in the objective function, default to 0.0001
- `NAFac`: the scaling factor for the NA term in the objective function, default to 1
- `popSize`: the population size for the genetic algorithm, default set to 50
- `pMutation`: the mutation probability for the genetic algorithm, default set to 0.5
- `maxTime`: the maximum optimisation time in seconds, default set to 60
- `maxGens`: the maximum number of generations in the genetic algorithm, default set to 500
- `stallGenMax`: the maximum number of stall generations in the genetic algorithm, default to 100
- `selPress`: the selective pressure in the genetic algorithm, default set to 1.2
- `elitism`: the number of best individuals that are propagated to the next generation in the genetic algorithm, default set to 5
- `relTol`: the relative tolerance for the best bitstring reported by the genetic algorithm, i.e., how different from the best solution, default set to 0.1
- `verbose`: logical (default to TRUE) do you want the statistics of each generation to be printed on the screen?
- `priorBitString`: At each generation, the GA algorithm creates a population of bitstrings that will be used to perform the optimisation. If the user knows the values of some bits, they can be used to overwrite bit values proposed by the GA algorithm. If provided, the priorBitString must have the same length as the initial bitstring and be made of 0, 1 or NA (by default, this bitstring is set to NULL, which is equivalent to setting all bits to NA). Bits that are set to 0 or 1 are used to replace the bits created by the GA itself (see example).
- `timeIndex`: the index of the time point to optimize. Must be greater or equal to 2 (1 corresponds to time=0). Must be less than the number of time points. Default is 2.
Details

The whole procedure is described in details in Saez-Rodriguez et al. (2009). The basic principle is that at each generation, the algorithm evaluates a population of models based on excluding or including some gates in the initial pre-processed model (this is encoded in a bitstring with contains 0/1 entries for each gate). The population is then evolved based on the results of the evaluation of these networks, where the evaluation is obtained by simulating the model (to steady state) under the various conditions present in the data, and then computing the squared deviation from the data, to which a penalty is added for size of the model and for species in the model that do not reach steady state.

Value

This function returns a list with elements:

- **bString**: the best bitstring
- **bScore**: the best score
- **results**: a matrix with columns "Generation","Best_score","Best_bitString","Stall_Generation","Avg_Score_Gen","Best_score_Gen","Best_bit_Gen","Iter_time"
- **stringsTol**: the bitstrings whose scores are within the tolerance
- **stringsTolScores**: the scores of the above-mentioned strings

Author(s)

C. Terfve, T. Cokelaer

References


See Also

gabinaryTN, simulatorT1

Examples

data(CNOlistToy,package="CellNOptR")
data(ToyModel,package="CellNOptR")

# pre-process model
model = preprocessing(CNOlistToy, ToyModel)

# optimise
initBstring<-rep(1,length(model$reacID))
ToyT1opt<-gaBinaryT1(
CN0list=CNOlistToy,
model=model,
initBstring=initBstring,
maxGens=100, popSize=10, verbose=FALSE)

# During the optimisation, some bits can be overwritten by your prior knowledge
# First, you need to create a priorBitString made of NA where known bit values
# are replaced by 0 or 1
priorBitString = rep(NA, length(model$reacID))
priorBitString[1] = 0
priorBitString[2] = 1

# Second, you call the gaBinaryT1 function by providing the priorBitString
# argument:
ToyT1opt<-gaBinaryT1(CNOlist=CNOlistToy, model=model,
  initBstring=initBstring,maxGens=10, popSize=10, verbose=FALSE,
  priorBitString=priorBitString)

---

### Description

This is the genetic algorithm for time point N, that should follow optimisation based on time point 1.

Replaces gaBinaryT2 since version 1.3.28

### Usage

```r
gaBinaryTN(CNOlist, model, bStrings, sizeFac = 1e-04, NAFac = 1,
  popSize = 50, pMutation = 0.5, maxTime = 60, maxGens = 500,
  stallGenMax = 100, selPress = 1.2, elitism = 5, relTol = 0.1, verbose=TRUE,
  priorBitString=NULL, timeIndex = NULL)
```

### Arguments

- **CNOlist**: a CNOlist on which the score is based (based on valueSignals[[3]], i.e. data at t2)
- **model**: a model structure, as created by readSIF, normally pre-processed but that is not a requirement of this function
- **bStrings**: the optimal bitstring from optimisation at time 1 (i.e. a vector of 0s and 1s)
- **sizeFac**: the scaling factor for the size term in the objective function, default to 0.0001
- **NAFac**: the scaling factor for the NA term in the objective function, default to 1
- **popSize**: the population size for the genetic algorithm, default set to 50
- **pMutation**: the mutation probability for the genetic algorithm, default set to 0.5
- **maxTime**: the maximum optimisation time in seconds, default set to 60
- **maxGens**: the maximum number of generations in the genetic algorithm, default set to 500
- **stallGenMax**: the maximum number of stall generations in the genetic algorithm, default to 100
- **selPress**: the selective pressure in the genetic algorithm, default set to 1.2
- **elitism**: the number of best individuals that are propagated to the next generation in the gen. al. default set to 5
- **relTol**: the relative tolerance for the best bitstring reported by the genetic algorithm, i.e.how different from the best solution can solutions be to be reported as well, default set to 0.1
verbose logical (default to TRUE) do you want the statistics of each generation to be printed on the screen

priorBitString A bitString of same length at the initial bitstring made of 0, 1 or NA. By default, this bitstring is set to NULL (equivalent to setting all bits to NA). If provided, all bitstring in a population will be changed to be in agreement with the priorBitString list.

timeIndex todo

Details
This function takes in the same input as the T1 ga, but in addition it takes in the bitstring optimised for T1, and does not take an initial bitstring. Be aware that the bitString that this function returns is one that only includes the bits that it actually looks at, i.e. the bits that were 0 in the bStringT1

Value
This function returns a list with elements:
- bString the best bitstring
- results a matrix with columns "Generation","Best_score","Best_bitString","Stall_Generation","Avg_Score_Gen","Best_score_Gen","Best_bit_Gen","Iter_time"
- stringsTol the bitstrings whose scores are within the tolerance
- stringsTolScores the scores of the above-mentionned strings

Author(s)
C.Terfve, T. Cokelaer

See Also
getFit, simulatorT1, simulatorT2, gaBinaryT2

Examples

```r
#load data
data(CNOlistToy2,package="CellNOptR")
data(ToyModel2,package="CellNOptR")

#pre-process model
checkSignals(CNOlistToy2,ToyModel2)
model = preprocessing(CNOlistToy2, ToyModel2)

#optimise t1
ToyT1<-gaBinaryT1(
CNOlist=CNOlistToy2,
model=model,
maxGens=10,
popSize = 10,
verbose=FALSE)

#Optimise T2
```
ToyT2<-gaBinaryTN(
    CNOlist=CNOlistToy2,
    model=model,
    bStrings=list(ToyT1$bString),
    maxGens=10,
    popSize = 10,
    verbose=FALSE)

getFit

**getFit**

*Compute the score of a model*

**Description**

This function computes the value of the objective function for a model and an associated data set, as a sum of a term that computes the fit of model to data, a term that penalises the NA values produced by the model, and a term that penalises increasing size of the model.

**Usage**

```r
getFit(simResults, CNOlist, model, indexList=NULL, timePoint=c("t1", "t2"), sizeFac=1e-04, NAFac=1, nInTot, simResultsT0=NULL)
```

**Arguments**

- `simResults`: matrix of simulated results (the full one as output by the simulator)
- `CNOlist`: a CNOlist to compare the simulated results with
- `model`: a model that has already been cut to contain only the reactions in the optimal bitstring
- `indexList`: list of indexes as produced by indexFinder. User should not use this parameter that is kept for back compatibility with previous version of the simulator written in R. The new simulator (C code) does not necessitate the usage of the indexList parameter in this function anymore.
- `timePoint`: "t1" or "t2" tells which time point we are looking at. If `timePoint="t1"` then we will compare the `simResults` to the results stored in `CNOlist$valueSignals[[2]]`. If `timePoint="t1"` then we will compare the `simResults` to the results stored in `CNOlist$valueSignals[[2]]`
- `sizeFac`: weights the penalty for the size of the model, default=0.0001
- `NAFac`: weights the penalty for the number of NAs
- `nInTot`: the number of inputs in the model prior to cutting, used to normalised the size penalty
- `simResultsT0`: Results of the time 0 simulator (internal usage of gaBinaryT1)

**Details**

BE AWARE: contrary to what is done in the Matlab version of CellNOpt, here the simulation results are computed beforehand and the model that is input into this function is a model that has already been cut i.e. that only contains the reactions present in the optimised model (i.e. should be the same model as the one that you input into the simulator). Also, the `simResults` matrix is the full one as output by the simulator, i.e. it contains results for all species in the model, not only the signals.
Value

This function returns a single number, the value of the objective function.

Author(s)

C. Terfve

References


See Also

gaBinaryT1, simulatorT1

Examples

# Here we will evaluate the fit of the full initial model, without pre-processing or any optimisation

data(CNOlistToy, package="CellNOptR")
data(ToyModel, package="CellNOptR")

indicesToy<-indexFinder(CNOlistToy, ToyModel, verbose=FALSE)
ToyFields4Sim<-prep4sim(ToyModel)
simResults<-simulatorT1(
  CNOlist=CNOlistToy,
  model=ToyModel,
  simList=ToyFields4Sim,
  indexList=indicesToy)
simResults = simResults[, indicesToy$signals]
Score<-getFit(
  simResults=simResults,
  CNOlist=CNOlistToy,
  model=ToyModel,
  timePoint="t1",
  nInTot=length(which(ToyModel$interMat == -1))
)

graph2sif

Convert graph to SIF

Description

This function converts a network form graph format to SIF format. The resulting table can also be saved in a SIF file.

Usage

graph2sif(graph, writeSif=FALSE, filename="Graph")
indexFinder

Arguments

graph  a graph, as generated using sif2graph
writeSif  if writeSif=FALSE (default) the SIF file is not saved. If writeSif=TRUE it is saved.
filename  the name of the SIF file saved if writeSif=TRUE. Default is Model.sif.

Details

The sign of link is supposed to be encoded in the graph as the weight of the edge (-1 negative regulation, +1 positive regulation).

Value

sifFile  a table with all the links in the model in the format sourceNode-tab-sign-tab-targetNode

Author(s)

F. Eduati

See Also

model2sif, sif2graph, readSIF.

Description

This function finds the indices, in the model fields, of the species that are measured/inhibited/stimulated. It looks for their position in model$namesSpecies which has the same order as the rows of interMat and notMat, and therefore these indexes can be used there as well.

Usage

indexFinder(CNOlist, model, verbose=FALSE)

Arguments

CNOlist  a CNOlist structure, as produced by makeCNOlist
model  a model structure, as produced by readSIF
verbose  do you want information about the cues and signals identities printed on the screen? Default if false but we would advise to set it to true when the function is called for the first time.
Value

a list with fields:

- `signals` vector of indices of the measured species
- `stimulated` vector of indices of the stimulated species
- `inhibited` vector of indices of the inhibited species

Note

For internal usage since version 1.3.28

Author(s)

C. Terfve

See Also

`makeCNOlist`, `readSIF`

Examples

data(CNOlistToy, package = "CellNOptR")
data(ToyModel, package = "CellNOptR")
indicesToy <- indexFinder(CNOlistToy, ToyModel, verbose = TRUE)

---

**internals**

List of CellNOptR internal functions.

**Description**

This is a list of functions that are part of CellNOptR but are not exposed to the end-user. It may be of interest for developers. They may have a manual associated to it. If so, you can get the documentation in a R console as usual by tying preceding the name of the function with question tag.

**Details**

<table>
<thead>
<tr>
<th>Function</th>
<th>deprecated since</th>
<th>manual</th>
</tr>
</thead>
<tbody>
<tr>
<td>cSimulator</td>
<td>internal usage</td>
<td>yes</td>
</tr>
<tr>
<td>buildBitString</td>
<td>internal usage</td>
<td>yes</td>
</tr>
<tr>
<td>simulateT1</td>
<td>1.3.28 (use simulateTN)</td>
<td>yes</td>
</tr>
</tbody>
</table>

**Author(s)**

T.Cokelaer
LiverDREAM

Model used for the DREAM3 challenge

Description
This data object contains the model used in the package vignette, already loaded and formatted as a Model object. This is to be used with the data in "CNOListDREAM"

Usage
DreamModel

Format
DreamModel is a list with fields "reacID" (character vector), "namesSpecies" (character vector), "interMat" (numerical matrix), "notMat" (numerical matrix).

Source
This data and model is extracted from the Matlab version of CellNOpt1.0 (http://www.ebi.ac.uk/saezrodriguez/software.html#CellNetOptimizer).

References

makeCNOlist
Make a CNOlist structure

Description
This function takes as input the output of readMIDAS and extracts the elements that are needed in a CNO project. Instead, please use the CNOlist class to read a MIDAS file that will be converted to a CNOlist.

Usage
makeCNOlist(dataset, subfield, verbose=TRUE)

Arguments
dataset output of readMIDAS
subfield TRUE or FALSE, specifies if the column headers contain subfields or not i.e. if I should look for TR:sthg:sthg or just TR:sthg.
verbose logical (default to TRUE) print information on the screen.
Details

Be aware that most of the functions in this package, including this one, expect the data to contain measurements at time 0, but these should all be equal to zero according to the normalisation procedure that should be used. Therefore, if you have one time point, the files valueSignals contains two matrices, one for t0 and one for t1.

If there are replicate rows in the MIDAS file (i.e., identical cues and identical time), this function averages the values of the measurements for these replicates.

Columns with the following tags are ignored: NOINHIB, NO-INHIB, NO-LIG, NOCYTO.

Value

a CNOlist with fields

- namesCues: a vector of names of cues
- namesStimuli: a vector of names of stimuli
- namesInhibitors: a vector of names of inhibitors
- namesSignals: a vector of names of signals
- timeSignals: a vector of times
- valueCues: a matrix of dimensions nConditions x nCues, with 0 or 1 if the cue is present or absent in the particular condition
- valueInhibitors: a matrix of dimensions nConditions x nInhibitors, with 0 or 1 if the inhibitor is present or absent in the particular condition
- valueStimuli: of dimensions nConditions x nStimuli, with 0 or 1 if the stimuli is present or absent in the particular condition
- valueSignals: a list of the same length as timeSignals, each element containing a matrix of dimensions nConditions x nsignals, with the measurements.
- valueVariances: a list of the same length as timeSignals, each element containing a matrix of dimensions nConditions x nsignals, with the standard deviation of the replicates.

Author(s)

C. Terfve, T. Cokelaer

References


See Also

readMIDAS, CNOlist-class
Examples

tmpdir<-tempdir()
setwd(tmpdir)
cpfile<-(dir(system.file("ToyModel",package="CellNOptR"),full=TRUE)
file.copy(from=cpfile,to=getwd(),overwrite=TRUE)
dataToy<-readMIDAS(MIDASfile='ToyDataMMB.csv')
CNOlistToy<-makeCNOlist(dataset=dataToy,subfield=FALSE)

mapBack

Map an optimised model back onto the PKN model.

Description

Map an optimised model back onto the PKN model.

Usage

mapBack(model, PKN, bString)

Arguments

model the optimised model
PKN the Prior Knowledge network
bString the optimised bitString

Value

bStringPKN the corresponding bitstring corresponding to the original PKN.

Author(s)

F.Eduati

See Also

graph2sif, sif2graph, readSIF.
model2igraph  

**Convert a model object to a igraph object**

**Description**

This function receives as input a model object and converts it to a graph object made by igraph. igraph provides lots of utilities especially to write the file in different format such as GML.

**Usage**

```r
model2igraph(model)
```

**Arguments**

- **model**
  - the model as generated using `readSIF`

**Value**

- **g**
  - a igraph object

**Author(s)**

T. Cokelaer

**See Also**

`graph2sif`, `sif2graph`

---

model2sif  

**Convert a model object in sif format**

**Description**

This function receives as input a model object and converts it to the cytoscape sif format. It can be used to convert either the whole model (before or after pre-processing) or the optimized one (if the corresponding bitString in provided). The resulting table can also be saved in a sif file.

**Usage**

```r
model2sif(model, optimRes=NA, writeSif=FALSE, filename="Model")
```

**Arguments**

- **model**
  - the model as generated using `readSIF`
- **optimRes**
  - the output of the optimisation (as obtained using `gaBinaryT1`), default set to NA
- **writeSif**
  - if writeSif=FALSE (default) the sif file is not saved. If writeSif=TRUE it is saved.
- **filename**
  - the name of the sif file saved if writeSif=TRUE. Default is Model.sif.
normaliseCNOlist

Details

All links in the model are converted in sif format that is sourceNode-tab-sign-tab-targetNode. If there are ANDs, they are converted using dummy nodes called and# (e.g. A+B=C will be A-tab-1-tab-and1; B-tab-1-tab-and1; and1-tab-1-tab-C).

Value

sifFile a table with all the links in the model in the format sourceNode-tab-sign-tab-targetNode

Author(s)

F.Eduati

See Also

graph2sif, sif2graph, readSIF,

Description

This function takes in a CNOlist and does the normalisation of the data between 0 and 1, according to two different procedures (see details).

Usage

normaliseCNOlist(CNOlist, EC50Data=0.5, HillCoef=2, EC50Noise=0., detection=0, saturation=Inf, changeTh=0, norm2TorCtrl=NULL, mode="time", options=list(rescale_negative = T), verbose=FALSE)

Arguments

CNOlist a CNOlist
EC50Data parameter for the scaling of the data between 0 and 1, default=0.5
HillCoef Hill coefficient for the scaling of the data, default to 2
EC50Noise parameter for the computation of a penalty for data comparatively smaller than other time points or conditions. No effect if set to zero (default).
detection minimum detection level of the instrument, everything smaller will be treated as noise (NA), default to 0
saturation saturation level of the instrument, everything over this will be treated as NA, default to Inf.
changeTh threshold for relative change considered significant, default to 0
norm2TorCtrl deprecated since 1.5.0. Use the mode argument instead.
mode "time" or "ctrl" or "raw" (experimental): choice of a normalisation method: "ctrl" computes the relative change compared to the control at the same time. "time" computes the relative change compared to the same condition and measurement at time 0. "raw" does not take into account time zero data; data are relative to time 0 so can be positive or negative values.
normaliseCNOlist

options  rescale column with negative values to be in 0-1 range (experimental)
verbose  prints some information if True (default is False)

Details

The normalisation procedure works as follows:

1. every value that is out of the dynamic range of the equipment (as specified by the parameters detection and saturation) are set to NA,
2. values are transformed to fold changes relative to the same condition at t0 (if mode="time") or the control condition (i.e. same inhibitors, no stimuli) at the same time (if mode="ctrl"),
3. the fold changes are transformed with a Hill function
   \[ \frac{x^{\text{HillCoef}}}{(EC_{50}\text{Data}^{\text{HillCoef}})+x^{\text{HillCoef}}} \]
4. a penalty for "noisiness" is computed for each measurement as the value divided by the maximum value for that readout across all conditions and times (excluding values out of the dynamic range)
5. the noise penalty is transformed by a saturation function (for each measurement)
   \[ \frac{x}{(EC_{50}\text{Noise}+x)} \]
6. the noise penalty and Hilled fold changes are multiplied,
7. if the fold change is negative and bigger than ChangeTh, the resulting product is multiplied by -1, if the fold change is smaller than ChangeTh (either positive or negative), it is set to 0.

The normalisation procedure applied here is explained in details in saez-Rodriguez et al. (2009).

As the normalisation procedure works by computing a fold change relative to the same condition at time 0 or the control condition, if the aforementioned conditions have a value of zero (which is not expected with any common biochemical technique), then the fold change calculation will return a "NaN" value. If this is a problem for your particular case then we would suggest putting a dummy, very low value, instead of the zero, or setting that measurement to "NA" in the MIDAS file.

Value

a normalised CNOlist

Author(s)

C. Terfve

References


See Also

makeCNOlist
Examples

#Load a CNOlist
data(CNOlistToy, package="CellNOptR")

#Replace the values in the list by random values
#(for demonstration purposes, when actually using this function you would simply load a non-normalised CNOlist)

CNOlistToy$valueSignals$t0<-matrix(  
data=runif(n=(dim(CNOlistToy$valueSignals$t0)[1]*dim(CNOlistToy$valueSignals$t0)[2]), min=0, max=400),  
nrow=dim(CNOlistToy$valueSignals$t0)[1],  
ncol=dim(CNOlistToy$valueSignals$t0)[2])

CNOlistToy$valueSignals[[2]]<-CNOlistToy$valueSignals[[1]]+matrix(  
data=runif(n=(dim(CNOlistToy$valueSignals$t0)[1]*dim(CNOlistToy$valueSignals$t0)[2]), min=0, max=100),  
nrow=dim(CNOlistToy$valueSignals$t0)[1],  
ncol=dim(CNOlistToy$valueSignals$t0)[2])

CNOlistToyN<-normaliseCNOlist(  
CNOlistToy,  
EC50Data = 0.5,  
HillCoef = 2,  
EC50Noise = 0.1,  
detection = 0,  
saturation = Inf,  
changeTh = 0,  
mode = "time")

plot-method

plot a "CNOlist" object - methods

Description

A plot method for CNOlist.

Usage

signature(x="CNOlist"): Please see the help page for the plot.CNOlist method in the CellNOptR package

arguments

  x  The CNOlist object to plot

Author(s)

  T.Cokelaer

See Also

  readMIDAS, makeCNOlist
plotCNOlist

Plot the data in a CNOlist

Description

This function plots the data in a CNOlist as a matrix of plots with a row for each condition and a column for each signal, and an extra plot for each row that specifies which cues are present.

Usage

plotCNOlist(CNOlist)

Arguments

CNOlist

a CNOlist

Details

This function can plot the normalised values or the un-normalised ones, it just needs a CNOlist.

Value

This function just produces a plot on your graphics window

Author(s)

C. Terfve

See Also

plotCNOlistPDF, plotCNOlistLarge, plotCNOlistLargePDF

Examples

data(CNOlistToy, package="CellNOptR")
plotCNOlist(CNOlistToy)
plotCNOlist2 Another version of plotCNOlist that allows to plot 2 cnolist in the same
layout to compare them. This function uses ggplot2 library. It is rec-
mommended for small data sets (about 15 species).

Description

This function plots the data in a CNOlist as a matrix of plots with a row for each condition and a
column for each signal. Cues are simply represented by a number.

Usage

plotCNOlist2(cnolist, simulated_cnolist=NULL, ymin=0,ymax=1)

Arguments

cnolist a CNOlist
simulated_cnolist another cnolist
ymin Change the lower y-limit (default is 0)
ymax Change the lower y-limit (default is 1)

Details

This function can plot either a single CNOlist, or 2 on top of each other.

Author(s)

T. Cokelaer

See Also

plotCNOlistPDF, plotCNOlistLarge, plotCNOlistLargePDF, plotCNOlist

Examples

# this data set is not an object so we need to convert it
data(CNOlistToy,package="CellNOptR")
cnolist = CNOlist(CNOlistToy)
plotCNOlist2(cnolist)
plotCNOlistLarge

Plot the data in a CNOlist, for lists with many conditions.

Description

This function plots the data in a CNOlist as a matrix of plots with a row for each condition and a column for each signal, and an extra plot for each row that specifies which cues are present.

Usage

plotCNOlistLarge(CNOlist, nsplit=4, newDevice=FALSE)

Arguments

CNOlist

a CNOlist

nsplit

the number of splits in the condition dimension (one new plot window will be produced for each split, i.e. if you have 80 conditions and specify 4 splits you will get 4 plots with 20 conditions each).

newDevice

nsplit plots are created within the same device. In principle, most of the R Graphical User Interface will allow the user to navigate between the different plots. However, if scripting only the last plot will be seen. If you want to create new device for each different plot, then set this option to TRUE.

Details

This function can plot normalised values or the un-normalised ones, it just needs a CNOlist. This function makes plots of CNOlists that are more readable when many conditions are present in the data. In addition to plotting the conditions divided into multiple plots, this function also plots the cues divided in two columns, one for inhibitors and one for stimuli.

Value

This function just produces plots on your graphics window.

Author(s)

C. Terfve

See Also

plotCNOlist, plotCNOlistPDF, plotCNOlistLargePDF

Examples

data(CNOlistDREAM, package="CellNOptR")
plotCNOlistLarge(CNOlistDREAM, nsplit=2)
plotCNOlistLargePDF

Plots a CNOlist into a pdf file, for lists with many conditions.

Description
This function is a wrapper for plotCNOlistLarge, that plots the output directly in a pdf file.

Usage
plotCNOlistLargePDF(CNOlist, filename, nsplit, width=14, height=7)

Arguments
- CNOlist: a CNOlist
- filename: a name for your pdf file, eg. "plot.pdf"
- nsplit: the number of splits along the condition dimension (see plotCNOlistLarge)
- width: set the width of the PDF document.
- height: set the height of the PDF document.

Details
This function makes plots of CNOlists that are more readable when many conditions are present in the data. In addition to plotting the conditions divided into multiple plots, this function also plots the cues divided in two columns, one for inhibitors and one for stimuli.

Value
This function doesn’t return anything, it just produces a pdf file with your plots, in your current working directory.

Author(s)
C. Terfve

See Also
plotCNOlistLarge, plotCNOlist, plotCNOlistPDF

Examples
```
tmpdir<-tempdir()
setwd(tmpdir)
data(CNOlistDREAM, package="CellNOptR")
plotCNOlistLargePDF(CNOlistDREAM, filename="dreamData.pdf", nsplit=2)
```
plotCNOListPDF  
Plots a CNOList into a pdf file.

Description
This function is a wrapper for plotCNOList, that plots the output directly in a pdf file.

Usage
plotCNOListPDF(CNOList, filename)

Arguments
- **CNOList**: a CNOList
- **filename**: a name for your pdf file, eg. "plot.pdf"

Value
This function doesn’t return anything, it just produces a pdf file containing your plot, in your working directory.

Author(s)
C. Terfve

See Also
plotCNOList, plotCNOListLarge, plotCNOListLargePDF

Examples
```r
tmpdir<-tempdir()
setwd(tmpdir)
data(CNOListToy,package="CellNOptR")
plotCNOListPDF(CNOList=CNOListToy,filename="ToyModelGraph.pdf")
```

plotFit  
Plot the evolution of an optimisation

Description
This function takes in the results of an optimisation by gaBinaryT1 and plots the evolution of best fit and average fit against generations.

Usage
plotFit(optRes, filename = NULL)
plotModel

Arguments

optRes an object created by the optimisation engine (gabinaryT1)
filename NULL or string: if provided, the plot is save in PDF format in the filename.

Value

This function doesn’t return anything, it just produces a plot in your graphics window.

Author(s)

C. Terfve

See Also

gaBinaryT1

Examples

data(CNOlistToy, package="CellNOptR")
data(ToyModel, package="CellNOptR")

#process the model
model = preprocessing(CNOlistToy, ToyModel)

#optimise
ToyT1opt<-gaBinaryT1(
  CNOlist=CNOlistToy,
  model=model,
  maxGens=10,
  popSize=10,
  verbose=FALSE)

plotFit(optRes=ToyT1opt)

plotModel

Plot a model

Description

This function can be used to plot a prior model network before any pre-processing step. However, additional information can be provided such as a CNOlist (see makeCNOlist and readMIDAS) or information related to the pre-processing steps (compression, NONC nodes, expansion gates). It can also be used to plot optimised model given the optimisation bitstring.

Usage

plotModel(model, CNOlist=NULL, bString=NULL, indexIntegr=NULL, signals=NULL, stimuli=NULL, inhibitors=NULL, NCNO=NULL, compressed=NULL, output="STDOUT", filename=NULL, graphvizParams=list(), show=TRUE, remove_dot=TRUE)
Arguments

model a model as returned by `readSIF`. Alternatively, the filename can also be provided.

CNOlist output of `makeCNOlist`

bString a sequence made of numbers between 0 and 1 of same length as the one returned by the Genetic Algorithm (GA). This is a generalisation of the bitString returned by the GA function: several bit strings can be averaged and used.

indexIntegr additional indices to highlight some edge (optional).

signals a list of nodes belonging to the signals class

stimuli a list of nodes belonging to the stimuli class

inhibitors a list of nodes belonging to the inhibitors class

NCNO a list of NCNO nodes.

compressed a list of compressed nodes

filename the filename (without extension) used to write the dot file

output the type of output (PNG, PDF, SVG accepted)

graphvizParams a list of optional arguments dedicated to Rgraphviz to tune the layout:
  • arrowsize default is 2
  • sizea string for the size of the dot output; default is "15,15"
  • fontsize default is 22
  • edgecolor default is "black"
  • nodeLabels overwrit node label with a list of proper length.
  • nodeWidth default is 2
  • nodeHeight default is 1
  • viewEmptyEdges default is TRUE
  • mode can be 'classic' or 'sbgn' (default). The difference appears in the and gate.
    • andWidth = 0.2 in 'classic' mode and 0.5 in 'sbgn' mode
    • andHeight = 0.2 in 'classic' mode and 0.5 in 'sbgn' mode

show show the plot (default is True)

remove_dot remove the dot file that has been created (default if False)

Details

This function plots the model and also saves it in a dot file that can be processed later on. However, you can also save the plot in PNG or PDF or SVG format (one at a time).

The CNOlist argument contains the signals/stimuli/inhibitors so if you provide a CNOlist there is no need to use these arguments. If you decide to use them they will overwrite the contents of the CNOlist argument.

optimRes is the output of `gaBinary`. One of its field is called bString and contains a list of 0 and 1 (the optimisation is performed with a binary procedure). This list of 0 and 1 is then used to plot or not the edges of the model. However, you can provide a bitString made of floats (e.g., average of several bitStrings). In such case, edges will appear in gray light or dark according to the bistring value (between 0 and 1).
### plotOptimResults

**Value**

- A graph representation of the model

\$graph\$g  
\$graph\$attrs  
\$graph\$nodeAttrs  
\$graph\$edgeAttrs  
\$graph\$clusters

**Note**

This function depends on the Rgraphviz package.

**Author(s)**

T. Cokelaer

**See Also**

readMIDAS, readSIF, makeCNOlist, writeNetwork, writeDot, gaBinaryT1

**Examples**

```r
data(CNOlistToy, package="CellNOptR")
data(ToyModel, package="CellNOptR")
res <- plotModel(ToyModel, CNOlist=CNOlistToy, compressed=c("TRAF6", "p38"),
                 graphvizParams=list(mode="classic", fontsize=30))
```

---

**plotOptimResults**  
*Plot the data and simulated values*

**Description**

This function is the equivalent of CNOPlotFits, it plots the data and the simulated values, along with an image plot that tells which cues were present. The plots are coloured according to the fit between data and simulated data.

**Usage**

`plotOptimResults(simResults, expResults, times, namesCues, namesSignals, valueCues, formalism="new")`
Arguments

- **simResults**: a list with a field for each time point, each containing a matrix of dimensions (number of conditions) \( \times \) (number of signals), with the first field being \( t_0 \). Typically produced by simulating a model and then extracting the columns that correspond to signals.

- **expResults**: same as above, but contains the experimental results, i.e., this is `CNOlist$valueSignals`.

- **times**: a vector of times, its length should be the same as the number of fields in `simResults` and `expResults`.

- **namesCues**: a vector of names, typically `CNOlist$namesCues`.

- **namesSignals**: a vector of names, typically `CNOlist$namesSignals`.

- **valueCues**: a matrix of dimensions (number of conditions) \( \times \) (number of cues), typically `CNOlist$valueCues`.

- **formalism**: New convention is to take the time=0 data set into account to compute the MSE. You can use the previous convention by setting this argument to something different from the default value.

Details

The colouring of the background is done as follows: the mean absolute difference between observed and simulated values are computed, and colours are chosen based on this value: red (above 0.9), indianred1 (between 0.8 and 0.9), lightpink2 (between 0.7 and 0.8), lightpink (between 0.6 and 0.7), mistyrose (between 0.5 and 0.6), palegoldenrod (between 0.4 and 0.5), palegreen (between 0.3 and 0.4), darkolivegreen3 (between 0.2 and 0.3), chartreuse3 (between 0.1 and 0.2), forestgreen (between 0 and 0.1). This function is used inside `cutAndPlotResultsT1`.

Value

This function doesn’t return anything, it just produces a plot in your graphics window.

Author(s)

C. Terfve

References


See Also

- `cutAndPlotResultsT1`

Examples

```r
tmpdir<-tempdir()
setwd(tmpdir)

# We will plot the fit of the full initial model compared to the data, without any optimisation
# This is normally not done on a stand alone basis, but if you have a model and would like to visualise its output

# load and prepare data
```
data(CNOlistToy,package="CellNOptR")
data(ToyModel,package="CellNOptR")
indicesToy<-indexFinder(CNOlistToy,ToyModel,verbose=TRUE)
ToyFields4Sim<-prep4sim(ToyModel)

#simulate model
simRes<-simulatorT1(CNOlist=CNOlistToy,model=ToyModel, simList=ToyFields4Sim, indexList=indicesToy)

#format data and results
simResults<-list(t0=matrix(data=0,nrow=dim(simRes)[1],ncol=dim(simRes)[2]),t1=simRes)
expResults<-list(t0=CNOlistToy$valueSignals[[1]],t1=CNOlistToy$valueSignals[[2]])

#plot
plotOptimResults(
simResults=simResults,
expResults=expResults,
times=CNOlistToy$timeSignals[1:2],
namesCues=CNOlistToy$namesCues,
namesSignals=CNOlistToy$namesSignals,
valueCues=CNOlistToy$valueCues)

---

**plotOptimResultsPan**  
Plots the data and simulated values from any CellNOptR formalism

**Description**

This function plots the data and simulated values according to each experiment in CNOlist. The data is shown as black triangles and the simulation by a blue dashed line. The combination of cues is given by a panel where black denotes the presence and white the absence of the cue. The goodness-of-fit between model and data is color-coded on a continuous scale from white to red.

**Usage**

```
plotOptimResultsPan(simResults, yInterpol=NULL, xCoords=NULL, CNOlist=CNOlist, formalism=c("ss1","ss2","ssN","dt","ode"), pdf=FALSE, pdfFileName="", tPt=NULL, plotParams = list(margin = 0.1, width=15, height=12, cmap_scale=1, cex=1.6, ymin=NULL))
```

**Arguments**

- **simResults**: A list with a field for each time point, each containing a matrix of dimensions (number of conditions) * (number of signals), with the first field being t0. Typically produced by simulating a model and then extracting the columns that correspond to signals.
- **yInterpol**: If using CNORdt, these are the interpolated experimental results from getFitTimeScale() that are needed to compare against the Boolean simulation.
These are the x-coordinates obtained from the optimized scaling factor in CNORdt that allow for comparison between time course experimental data and a Boolean model.

A CNOlist.

An abbreviation of the CellNOptR formalism being used.

A Boolean argument denoting whether to print the figure produced by this function to file.

If printing to file, the filename to be used.

The number of time points in the data.

A list of option related to the PDF and plotting outputs. Currently, the following attributes are used: (1) margin of the boxes, (2) width and height used while creating the PDF, (3) cmap_scale a value that scales the colors towards small errors (<1) or large errors (>1); default is 1 (linear colormap) (4) cex is the fontsize used in the header (5) ymin sets the minimum y axis limit; by default it is the minimum value found over all data points and therefore can be negative.

Depending on the logic formalism, this function is generally called from cutAndPlotResults*(). As shown in the example below however, it can plot the fit of any data and corresponding compatible model. The color denotes the goodness-of-fit, where white shows no difference between simulation and data and red is the maximum error from all conditions and readouts.

This function does not return a value.

A. MacNamara


See Also

cutAndPlotResultsT1

data(CNOlistToy, package="CellNOptR")
data(ToyModel, package="CellNOptR")
indicesToy <- indexFinder(CNOlistToy, ToyModel, verbose=TRUE)
ToyFields4Sim <- prep4sim(ToyModel)

# simulate model
simRes <- simulatorT1(CNOlist=CNOlistToy, model=ToyModel, simList=ToyFields4Sim, indexList=indicesToy)
simRes = simRes[, indicesToy$signals]
# format data and results
simResults <- list(t0=matrix(data=0, nrow=dim(simRes)[1], ncol=dim(simRes)[2], t1=simRes)
# plot
plotOptimResultsPan(simResults,
  CNOlist=CNOlistToy,
  formalism="ss1",
  pdf=FALSE,
  tPt=t0
)

---

plotOptimResultsPDF  *Plot the data and simulated values in a pdf file*

---

**Description**

This is a wrapper for plotOptimResults

**Usage**

plotOptimResultsPDF(simResults, expResults, times, namesCues, namesSignals, valueCues, filename, formalism="new")

**Arguments**

- `simResults`: a list with a field for each time point, each containing a matrix of dimensions number of conditions * number of signals, with the first field being t0. Typically produced by simulating a model and then extracting the columns that correspond to signals.
- `expResults`: same as above, but contains the experimental results, ie this is CNOlist$valueSignals.
- `times`: a vector of times, its length should be the same as the number of fields in simResults and ExpResults.
- `namesCues`: a vector of names, typically CNOlist$namesCues.
- `namesSignals`: a vector of names, typically CNOlist$namesSignals.
- `valueCues`: a matrix of dimensions (number of conditions) * (number of cues), typically CNOlist$valueCues.
- `filename`: a name for your file, eg. "plot.pdf".
- `formalism`: New convention is to take the time=0 data set into account to compute the MSE. you can use the previous convention by setting this argument to something different from the default value.

**Details**

The coloring of the background is done as follows: the mean absolute difference between observed and simulated values are computed, and colours are chosen based on this value: red (above 0.9), indianred1 (between 0.8 and 0.9), lightpink2 (between 0.7 and 0.8), lightpink (between 0.6 and 0.7), mistyrose (between 0.5 and 0.6), palegoldenrod (between 0.4 and 0.5), palegreen (between 0.3 and 0.4), darkolivegreen3 (between 0.2 and 0.3), chartreuse3 (between 0.1 and 0.2), forestgreen (between 0 and 0.1). This function is used inside cutAndPlotResultsT1.
prep4sim

Prepare a model for simulation

Description

Adds to the model some fields that are used by the simulation engine.
prep4sim

Usage

prep4sim(model)

Arguments

model a model list, as output by readSIF, normally pre-processed but that is not a requirement of this function

Details

This adds fields that are necessary for the simulation engine in a version that is extensible for constrained Fuzzy logic extension of the methods applied here (in development).

Value

this function returns a list with fields:

- finalCube stores, for each reac(row) the location of its inputs (col)
- ixNeg stores, for each reac(row) and each input (col) whether it is a negative input
- ignoreCube logical matrix of the same size as the 2 above, that tells whether the particular cell is filled or not
- maxIx row vector that stores, for each reac, the location of its output
- modelname stores the name of the model from which these fields were derived
- maxInput stores the max number of inputs observed in the model for a single reaction

Note

For internal usage since version 1.3.28

Author(s)

C. Terfve, T. Cokelaer

See Also

simulatorT1

Examples

data(ToyModel, package="CellNOptR")
ToyFields4Sim<-prep4sim(ToyModel)
### preprocessing

**Performs the pre-processing steps**

### Description

This function performs any of the following preprocessing steps:

1. removes Non-Controllable and Non-Observables nodes
2. compress the model
3. and-gates expansion

### Usage

```r
call = preprocessing(data, model, cutNONC=TRUE, compression=TRUE, expansion=TRUE, ignoreList=NA, maxInputsPerGate=2, verbose=TRUE)
```

### Arguments

- **data**
  - the CNOlist that contains the data that you will use

- **model**
  - the model object as returned by `readSIF`

- **cutNONC**
  - Removes the NONC nodes using `cutNONC` and `findNONC` (Default is TRUE).

- **compression**
  - Compress the model using `compressModel` (Default is TRUE).

- **expansion**
  - Add and gates using `expandGates` (Default is TRUE).

- **ignoreList**
  - list of reactions indices to ignore in the expansion step.

- **maxInputsPerGate**
  - used by the `expandGates` function to set maximum inputs per and gates.

- **verbose**
  - verbose option (Default is TRUE).

### Details

The function can apply any or none of the pre-processing steps. It returns the new model and the indices returned by `indexFinder`.

### Value

the new model

### Author(s)

T. Cokelaer

### See Also

`readSIF`, `readMIDAS`, `cutNONC`, `findNONC`, `compressModel`, `expandGates`.

### Examples

```r
data(ToyModel, package="CellNOptR")
data(CNOlistToy, package="CellNOptR")
model = preprocessing(CNOlistToy, ToyModel, cutNONC=FALSE)
```
randomizeCNOlist

add noise to the data contained in a CNOlist.

Description

This function takes in a CNOlist and does the normalisation of the data between 0 and 1, according to two different procedures (see details).

Usage

randomizeCNOlist(cnolist, sd=0.1, minValue=0, maxValue=1, mode="gaussian")

Arguments

cnolist: a CNOlist

sd: standard deviation to be used when adding gaussian noise. Not used if mode is uniform.

minValue: When adding Gaussian noise, the result may be below the minValue (default 0). If so, the value is set to minValue.

maxValue: When adding Gaussian noise, the result may be above the maxValue (default 1). If so, the value is set to maxValue.

mode: The mode can be either 'gaussian', 'shuffle' or uniform'. In gaussian mode, a gaussian noise is added to the data. The mean parameter is the data and the standard deviation is defined by the sd parameter. In uniform mode, the data is simply replaced by values taken from a uniform distribution between 0 and 1. In 'shuffle' mode all rows and columns are shuffled.

Value

a noisy CNOlist

Author(s)

T. Cokelaer

Examples

data(CNOlistToyMMB, package="CellNOptR")
cnolist = CNOlistToyMMB
cnolist2 = randomizeCNOlist(cnolist, mode="uniform")

# a method called randomize is available in the CNOlist class so you could type:
cnolist2 = randomize(cnolist, mode="uniform")
**readMIDAS**  
*Reads in a CSV MIDAS file*

**Description**

This function takes in a single argument, the name of a CSV MIDAS file containing the data, and returns a list that contains all the elements to build a CNOlist. The output of this function should be used as input for `makeCNOlist`.

**Usage**

```r
readMIDAS(MIDASfile, verbose=TRUE)
```

**Arguments**

- **MIDASfile** a CSV MIDAS file (see details)
- **verbose** logical (default to TRUE).

**Details**

This function does not return a CNOlist, but the output of this function can be used directly into `makeCNOlist` to create one. The MIDAS file format is described in Saez-Rodriguez et al. (2008).

If you have all of the readouts measured at the same series of time points, you can specify a unique DA: column which must have the format "DA:ALL".

**Value**

This function returns a list with fields:

- **dataMatrix** matrix containing the data in the MIDAS file
- **TRcol** indexes of the columns that contain the treatments (excluding cell line)
- **DAcol** indexes of the columns that contain the data time points
- **DVcol** indexes of the columns that contain the actual values (measurements)

**Author(s)**

C.Terfve

**References**


**See Also**

`makeCNOlist`
**Examples**

```r
tmpdir<-tempdir()
setwd(tmpdir)
cpfile<-dir(system.file("ToyModel",package="CellNOptR"),full=TRUE)
file.copy(from=cpfile,to=getwd(),overwrite=TRUE)
dataToy<-readMIDAS(MIDASfile="ToyDataMMB.csv")
CNOlistToy<-makeCNOlist(dataset=dataToy,subfield=FALSE)
```

**readSBMLQual**  
*Read a SBMLQual document and returns a SIF object (as returned by readSIG)*

**Description**

This function reads a SBMLQual XML file where a model is stored. The XML is scanned and saved in SIF format in a temporary file. This file is read by readSIF. The returned object is therefore the output of readSIF.

**Usage**

```r
readSBMLQual(filename)
```

**Arguments**

- `filename` The name of a SBMLQual file.

**Value**

A model list with fields:

- `interMat` contains a matrix with column for each reaction and a row for each species, with a -1 where the species is the source node and a +1 where the species is a target node, and 0 otherwise.

- `notMat` has the same format as `interMat` but just contains a 1 if the source node enters the reaction with a negative effect, and 0 otherwise.

- `namesSpecies` vector that contains the names of the species in the same order as the rows of the `interMat` and `notMat` matrices.

- `reacID` vector that holds character strings specifying the reaction in full letters, in the same order as the columns of `interMat` and `notMat` matrices.

**Author(s)**

T. Cokelaer

**References**

SBMLQual: qualitative models. See SBML.org for details.
Examples

```r
## Not run:
sif = readSBMLQual("test.xml")
## End(Not run)
```

### Description

This function reads in a cytoscape SIF file and creates a model object that can be used in the CellNOptR procedure.

### Usage

```r
readSIF(sifFile)
```

### Arguments

- `sifFile`: The name of a SIF file (Cytoscape format). See details for the accepted format.

### Details

The input argument is the name of a SIF file that contains a prior knowledge network. The SIF format (See http://wiki.cytoscape.org/Cytoscape_User_Manual/Network_Formats/) can be of the form:

```
nodeA typeA node2
```

or

```
node2 typeB node3 node4
```

with space or tabulations in between types and nodes. Spaces and tabulations have different meaning in the original cytoscape format. However, we do not differentiate them. Therefore names of the nodes cannot have white space inside them.

The accepted values for the types are -1 (inhibitor) or 1 (normal relation).

If there are ANDs they should be introduced as dummy nodes called "and#" (don’t forget the number after "and" otherwise this won’t be recognised). Please be aware that "and" nodes are not expected to be negated, i.e. there are not supposed to be !and1=xyz because that amounts to inverting the sign of all inputs of and1, which is more simply done at the inputs level.

The SIF format can also include unconnected node that is a row with a single name:

```
nodeA
```

Although there would be no error, these type of rows are ignored.
Value

a model list with fields:

interMat contains a matrix with column for each reaction and a row for each species, with a -1 where the species is the source node and a +1 where the species is a target node, and 0 otherwise

notMat has the same format as interMat but just contains a 1 if the source node enters the reac with a negative effect, and 0 otherwise

namesSpecies vector that contains the names of the species in the same order as the rows of the interMat and notMat matrices

reacID vector that holds character strings specifying the reaction in full letters, in the same order as the columns of interMat and notMat

Author(s)

C. Terfve

References


Examples

tmpdir<-tempdir()
setwd(tmpdir)
cpfile<-dir(system.file("ToyModel",package="CellNOptR"),full=TRUE)
file.copy(from=cpfile,to=getwd(),overwrite=TRUE)
ToyModel<-readSIF(sifFile="ToyPKNMMB.sif")

residualError

Compute the residual error for a dataset

Description

This function takes in a CNOlist and computes the residual error, which is the minimum error between the scaled continuous data and a binary boolean approximation of this data.

Usage

residualError(CNOlist)

Arguments

CNOlist a CNOlist

Details

Be aware that it is expected that$valueSignals[[1]] holds t0 (all signals=0) and $valueSignals[[2]] holds t1, $valueSignals[[3]] holds t2 and so on. The output is a list of residual errors at each time greater than 2. In addition, the total error is stored. For back compatibility, an additional field called t1andt2 is stored (NA is only t1 provided).
The function `sif2graph` receives as input a network in sif format and converts it to graph format.

**Usage**
```
sif2graph(sif)
```

**Arguments**
- `sif` : the name of a sif file or the equivalent table

**Details**
This function takes a network in sif format (table or file), i.e. `sourceNode-tab-sign-tab-targetNode`. If there are ANDs they should be introduced as dummy nodes called `and#` (don't forget the number after "and" otherwise this won't be recognised). Please be aware that "and" nodes are not expected to be negated, i.e. there are not supposed to be `!and1=xyz` because that amounts to inverting the sign of all inputs of `and1`, which is more simply done at the inputs level.

In the resulting graph, the sign of each link is encoded as the weight of the edge (-1 negative regulation, +1 positive regulation).

**Value**
- `g` : the corresponding graph

**Author(s)**
F. Eduati

**See Also**
- `graph2sif`, `model2sif`, `readSIF`
**simulateTN**  
**Cut and simulation of a boolean model at t1**

**Description**

This function cuts a model according to a bitstring optimised at T1, and simulates the model accordingly.

**Usage**

```r
simulateTN(CNOlist, model, bStrings)
```

**Arguments**

- `CNOlist`: a CNOlist object
- `model`: a full model
- `bStrings`: a bitstring to cut the model, as output by `gaBinaryT1` (i.e. a vector of 1s and 0s, of length equal to the number of reactions in the model)

**Details**

This function is a wrapper around the family of functions called `simulatorT1`, T2 and TN.

**Value**

A matrix of simulated values, including all species in the model, i.e. to be used as input of `gaBinaryTN`.

**Author(s)**

T.Cokelaer, S.Schrier based on `simulatorT1` (C.Terfve)

**See Also**

- `cutAndPlotResultsT1`, `simulatorT1`

**Examples**

```r
# This will compute the output of a random model obtained by randomly selecting  
# which gates of the initial models are included.

data(CNOlistToy, package="CellNOptR")
data(ToyModel, package="CellNOptR")

simRes<-simulateTN(  
  CNOlist=CNOlistToy,  
  model=ToyModel,  
  bStrings=list(round(runif(length(ToyModel$reacID)))))
```
simulatorT0

Simulation of a boolean model

Description
This is the simulator, inspired from BoolSimEngMKM in the Matlab CellNOpt, to be used on one time point simulations

Usage
simulatorT0(CNOlist, model, simList, indexList)

Arguments
- CNOlist: a CNOlist
- model: a model that only contains the reactions to be evaluated
- simList: a simList as created by prep4sim, that has also already been cut to contain only the reactions to be evaluated
- indexList: an indexList as created by indexFinder

Details
Differences from the BoolSimEngMKM simulator include: the valueInhibitors has not been previously flipped; the function outputs the values across all conditions for all species in the model, instead of only for the signal species. This is because then the output of this function can be used as initial values for the version of the simulator that works on time point 2 (not implemented in this version).

If you would like to compute the output of a model that contains some of the gates in the model but not all, we suggest that you use the function SimulateT1 and specify in the bStringT1 argument which gates you want to be included. Indeed, SimulateT1 is a wrapper around simulatorT0 that takes care of cutting the model for you before simulating it.

Value
This function outputs a single matrix of format similar to valueSignals in the CNOlist but that contains an output for each species in the model. This matrix is the simulated equivalent of valueSignals at time 1, if you consider only the columns given by indexSignals.

Author(s)
T. Cokelaer

References
**simulatorT1**

**See Also**

simulateTN, cutAndPlotResultsT1

**Examples**

#This computes the output of the full model, which is normally not done on a stand alone basis, but if you have
data(CNOlistToy,package="CellNOptR")
data(ToyModel,package="CellNOptR")

indicesToy<-indexFinder(CNOlistToy,ToyModel,verbose=TRUE)
ToyFields4Sim<-prep4sim(ToyModel)

Sim<-simulatorT0(
  CNOlist=CNOlistToy,
  model=ToyModel,
  simList=ToyFields4Sim,
  indexList=indicesToy)

---

**simulatorT1**  
*Simulation of a boolean model*

**Description**

This is the simulator, inspired from BoolSimEngMKM in the Matlab CellNOpt, to be used on one time point simulations

**Usage**

simulatorT1(CNOlist, model, simList, indexList, mode=1)

**Arguments**

- **CNOlist**  
a CNOlist
- **model**  
a model that only contains the reactions to be evaluated
- **simList**  
a simList as created by prep4sim, that has also already been cut to contain only the reactions to be evaluated
- **indexList**  
an indexList as created by indexFinder
- **mode**  
switch to use the cSimualor for time 0 or 1

**Details**

Differences from the BoolSimEngMKM simulator include: the valueInhibitors has not been previously flipped; the function outputs the values across all conditions for all species in the model, instead of only for the signal species. This is because then the output of this function can be used as initial values for the version of the simulator that works on time point 2 (not implemented in this version).

If you would like to compute the output of a model that contains some of the gates in the model but not all, we suggest that you use the function SimulateT1 and specify in the bStringT1 argument which gates you want to be included. Indeed, SimulateT1 is a wrapper around simulatorT1 that takes care of cutting the model for you before simulating it.
This function outputs a single matrix of format similar to valueSignals in the CNOList but that contains an output for each species in the model. This matrix is the simulated equivalent of valueSignals at time 1, if you consider only the columns given by indexSignals.

Author(s)

C. Terfve

References


Examples

```r
# This computes the output of the full model, which is normally not done on a stand alone basis, but if you have

data(CNOlistToy, package="CellNOptR")
data(ToyModel, package="CellNOptR")

indicesToy<-indexFinder(CNOlistToy, ToyModel, verbose=TRUE)
ToyFields4Sim<-prep4Sim(ToyModel)

Sim<-simulatorT1(
  CNOlist=CNOlistToy,
  model=ToyModel,
  simList=ToyFields4Sim,
  indexList=indicesToy)
```

## Description

This is the simulator at TN using a C implementation. The computation relies on the time TN-1. T1 is a special case that is solved by using `simulatorT2`.

## Usage

```r
simulatorTN(simResultsPrev, CNOlist, model, simList, indexList, timeIndex=3)
```
Arguments

- `simResultsPrev`: a matrix that is the output of `simulatorTN` (i.e. one row per condition and one column per species IN THE MODEL)
- `CNOlist`: a CNOlist
- `model`: a model that only contains the reactions to be evaluated
- `simList`: a simList as created by `prep4sim`, that has also already been cut to contain only the reactions to be evaluated
- `indexList`: an indexList as created by `indexFinder`
- `timeIndex`: 3 by default to behave like deprecated function `simulatorT2`. This is the timeIndex at which the simulation is requested.

Details

Differences from the BoolSimEngMKM simulator include: the `valueInhibitors` has not been previously flipped; the function outputs the values across all conditions for all species in the model, instead of only for the signal species. This is because then the output of this function can be used as initial values for the version of the simulator that works on time point 2 (not implemented in this version).

If you would like to compute the output of a model that contains some of the gates in the model but not all, we suggest that you use the function `SimulateT1` and specify in the `bStringT1` argument which gates you want to be included. Indeed, `SimulateT1` is a wrapper around `simulatorT1` that takes care of cutting the model for you before simulating it.

Value

This function outputs a single matrix of format similar to `valueSignals` in the CNOlist but that contains an output for each species in the model. This matrix is the simulated equivalent of `valueSignals` at time 1, if you consider only the columns given by `indexSignals`.

Author(s)

T. Cokelaer, based on `cSimulator` (A. MacNamara)

References


See Also

- `simulateTN`, `cutAndPlotResultsT1`
Examples

# This computes the output of the full model, which is normally not done on a stand alone basis, but if you have

data(CN0listToy,package="CellNOptR")
data(ToyModel,package="CellNOptR")

indicesToy<-indexFinder(CN0listToy,ToyModel,verbose=TRUE)
ToyFields4Sim<-prep4sim(ToyModel)

# Sim<-simulatorTN(
# CN0List=CN0listToy,
# model=ToyModel,
# simList=ToyFields4Sim,
# indexList=indicesToy)

ToyModel

DESCRIPTION

This data object contains the Toy model from the package vignette, already loaded and formatted as a Model object.

Usage

ToyModel

Format

ToyModel is a list with fields "reacID" (character vector), "namesSpecies" (character vector), "interMat" (numerical matrix), "notMat"(numerical matrix).

Source

This data and model is extracted from the Matlab version of CellNOpt1.0 (http://www.ebi.ac.uk/saezrodriguez/software.html#CellNetOptimizer).

References

Description

This data object contains the Toy model from the package vignette, already loaded and formatted as a Model object, and modified for the 2 time points version (a negative feedback between cJun and Jnk (!cJun=Jnk) is added).

Usage

ToyModel

Format

ToyModel is a list with fields "reacID" (character vector), "namesSpecies" (character vector), "interMat" (numerical matrix), "notMat" (numerical matrix).

Source

This data and model is extracted from the Matlab version of CellNOpt1.0 (http://www.ebi.ac.uk/saezrodriguez/software.html#CellNetOptimizer).

References


writeDot

Write a model, and attached features, to a dot file

Description

This function writes a model to a Graphviz dot file with encoded features such as edge weight and nodes status (see details).

Usage

writeDot(dotNodes,dotMatrix,model,filename)

Arguments

dotNodes internal variables created by writeNetwork or writeScaffold; dotNodes is a matrix with 2 columns: the first has the node names, and the second the attributes (signal, stimulated, inhibited, compressed, nano). A node can appear twice in this matrix if it belongs to more of one of the above categories; a node could also not appear here if it is is none of these categories


**writeDot**

**dotMatrix**
internal variables created by writeNetwork or writeScaffold; dotMatrix is a matrix with 4 or 5 columns, and a row for each reaction: the first column holds the name of the input node, the second column holds the sign of the reaction (-1 if negative, 1 if positive), the third column holds the name of the output node, the fourth column holds the time stamp (0,1,2), an optional 5th column holds the weights of the edges

**model**
A model to be plotted, if used inside writeNetwork then this should be the previous knowledge network (modelOriginal), if inside writeScaffold then this should be the scaffold (modelComprExpanded)

**filename**
a name for the file

**Details**
This function is not to be used on its own, it should be used internally to writeNetwork or writeScaffold. For the colouring of the nodes, nodes that are both stimulated and inhibited or any other combination, only one colour per category is used, and the following order of priority for the colours is used: signals prime over inhibited nodes which primes over stimulated nodes which primes over non-controllable/non-observable nodes, which primes over compressed. Nodes that are neither of those have a black contour, stimulated nodes are green, inhibited are red, measure are blue, compressed and non-controllable/non-observable nodes are black and dashed. Edges are coloured according to time stamp in the optimal model (green=t1, blue=t1 and/or t2, grey=neither); on the scaffold, the strokes of the edges reflects the weights in the models within reltol (i.e. for each edge, the weight is the frequency with which it appeared among the models within the relative tolerance boundaries around the best solution).

**Value**
This function does not have any output, it just writes a .dot file in your working directory.

**Author(s)**
C. Terfve

**References**

**See Also**
writeNetwork, writeScaffold

**Examples**

tmpdir<-tempdir()
setwd(tmpdir)

#load data
data(CNOlistToy,package="CellNOptR")
data(ToyModel,package="CellNOptR")

#pre-process model
indicesToy<-indexFinder(CNOlistToy,ToyModel,verbose=TRUE)
ToyNCNOindices<-findNONC(ToyModel,indicesToy,verbose=TRUE)
ToyNCNOcut<-cutNONC(ToyModel,ToyNCNOindices)
indicesToyNCNOcut<-indexFinder(CNOlistToy,ToyNCNOcut)
ToyNCNOcutComp<-compressModel(ToyNCNOcut,indicesToyNCNOcut)
indicesToyNCNOcutComp<-indexFinder(CNOlistToy,ToyNCNOcutComp)
ToyNCNOcutCompExp<-expandGates(ToyNCNOcutComp)

# optimise
ToyFields4Sim<-prep4sim(ToyNCNOcutCompExp)
initBstring<-rep(1,length(ToyNCNOcutCompExp$reacID))
ToyT1opt<-gaBinaryT1(
  CNOlist=CNOlistToy,
  model=ToyNCNOcutCompExp,
  initBstring=initBstring,
  maxGens=2,
  popSize=5,
  verbose=TRUE)

# write network
writeNetwork(
  modelOriginal=ToyModel,
  modelComprExpanded=ToyNCNOcutCompExp,
  optimResT1=ToyT1opt,
  optimResT2=NA,
  CNOlist=CNOlistToy)

---

writeMIDAS

Write a CNOlist structure into a MIDAS file

**Description**

This function takes a CNOlist structure (output of makeCNOlist and readMIDAS) and save it a MIDAS format.

**Usage**

writeMIDAS(CNOlist, filename, timeIndices=NULL, overwrite=FALSE)

**Arguments**

- **CNOlist**: a CNOlist structure
- **filename**: a filename. Not overwritten if it exists already
- **timeIndices**: select subset of the times to be saved. Works with indices (not time values)
- **overwrite**: overwrite the file if it exists already (Default is FALSE)

**Author(s)**

T. Cokelaer
writeNetwork

Write a previous knowledge network model to a sif file (with attribute files), as well as a dot file.

Usage

writeNetwork(modelOriginal, modelComprExpanded, optimResT1, optimResT2, CNOlist, tag = NULL, verbose=FALSE)

Arguments

modelOriginal  The PKN model
modelComprExpanded  The scaffold model (i.e. compressed and expanded)
optimResT1  The results of the optimisation process at t1
optimResT2  The results of the optimisation process at t2 (set this to NA if you have performed a one time point optimisation).
CNOlist  The CNOlist on which the optimisation is based
tag  NULL or string; tells whether you want to prefix filenames with a tag (replaces the default behaviour).
verbose  If verbose=TRUE, the function prints a message every time an edge in the scaffold network couldn’t be mapped back to the PKN

Description

This function writes the original previous knowledge network (the model that you loaded in the beginning of your analysis) in a sif file, with a nodes attribute file that specifies if each node was stimulated/inhibited/signal/compressed/non-controllable-non-observable and an edge attribute file that specifies if the edge was absent in the optimal model (0) present in the optimal model at t1 (1) or present in the optimal model at t2 (2).

This function also writes a Graphviz dot file that contains the same information (see writeDot for more information about the dot file conventions).

See Also

makeCNOlist, readMIDAS, CNOlist-class

Examples

tmpdir<-tempdir()
setwd(tmpdir)
data(CNOlistToy)
writeMIDAS(CNOlistToy, 'test.csv')
readMIDAS('test.csv')
writeMIDAS(CNOlistToy, 'test.csv', timeIndices=c(1,2), overwrite=TRUE)
writeNetwork

Details

The weights of the edges are computed as the mean across models within the relative tolerance limits, as output in the results from the optimisation $\text{stringsTol}$. Strings that are in $\text{stringsTol}$ are the ones that are within the relative tolerance limits around the best solution in the population across all generations of the optimisation.

If there is no time 2, then the argument optimResT2 should be = NA.

This function maps back the edges weights from the optimised (expanded and compressed) model to the original model. The mapping back only works if the path has length 2 at most (i.e. you have node1-comp1-comp2-node2, where comp refer to nodes that have been compressed).

Value

This function does not have any output, it just writes a sif file, an edge attribute file, and a node attribute file.

Note

The mapback of this function is still an open question, even in the Matlab version. Future developments will include more robust versions of the mapping back algorithm, probably as a separate mapback function.

Author(s)

C. Terfve

See Also

writeScaffold, writeDot

Examples

tmpdir<-tempdir()
setwd(tmpdir)

#load data
data(CNOlistToy, package="CellNOptR")
data(ToyModel, package="CellNOptR")

#pre-process model
indicesToy<-indexFinder(CNOlistToy,ToyModel,verbose=TRUE)
ToyNCNOindices<-findNONC(ToyModel,indicesToy,verbose=TRUE)
ToyNCNOcut<-cutNONC(ToyModel,ToyNCNOindices)
indicesToyNCNOcut<-indexFinder(CNOlistToy,ToyNCNOcut)
ToyNCNOcutComp<-compressModel(ToyNCNOcut,indicesToyNCNOcut)
indicesToyNCNOcutComp<-indexFinder(CNOlistToy,ToyNCNOcutComp)
ToyNCNOcutCompExp<-expandGates(ToyNCNOcutComp)

#optimise
ToyFields4Sim<-prep4sim(ToyNCNOcutCompExp)
initBstring<-rep(1,length(ToyNCNOcutCompExp$reacID))
ToyT1opt<-gaBinaryT1(...
writeReport

CNOlist=CNOlistToy,
model=ToyNCNoCutCompExp,
initBstring=initBstring,
verbose=TRUE,
maxGens=2,
popSize=5)

#write network
writeNetwork(
modelOriginal=ToyModel,
modelComprExpanded=ToyNCNoCutCompExp,
optimResT1=ToyT1opt,
optimResT2=NA,
CNOlist=CNOlistToy)

writeReport

Write a report of a CellNOptR analysis

Description
This function writes a short report of a CellNOptR analysis in an html page, that is linked to the various graphs produced.

Usage
writeReport(modelOriginal, modelOpt, optimResT1, optimResT2, CNOlist, directory,
namesFiles = list(dataPlot = NA, evolFitT1=NA, evolFitT2=NA, simResultsT1=NA, simResultsT2=NA, scaffold=NA, scaffoldDot=NA, tscaffold=NA, wscaffold=NA, PKN=NA, PKNdot=NA, wPKN=NA, nPKN=NA), namesData = list(CNOlist=NA, model=NA), resE=NULL)

Arguments
modelOriginal the original previous knowledge network (i.e. model that you loaded) in a model list format
modelOpt the model that was actually used for optimisation (i.e. the scaffold network, after compression and expansion) in a model list format
optimResT1 the results of the optimisation at t1, as output by gabinaryT1
optimResT2 the results of the optimisation at t2, as output by gabinaryT2. Set this to NA if you have performed a one time point optimisation.
CNOlist a CNOlist
directory the name of a new directory that will be created, where your results will be moved
namesFiles a list of the names of the files that should have been created. Depending on whether a t2 optimisation was performed or not, all or some of the following fields are expected: dataPlot, evolFitT1, evolFitT2, simResultsT1, simResultsT2, scaffoldDot, scaffold, tscaffold, wscaffold, PKN, PKNdot, wPKN, nPKN.
namesData a list with fields $CNOlist and $model that contain strings that are meaningful identifiers of your data and previous knowledge network (for your own record).
a vector with named entries t1, t2 and t3, as produced by the function `ResidualError`, that contains the residual error associated with the discretisation of the data. Since version 1.3.29, there is no need to provide this argument. Kept for back compatibility.

**Details**

Future versions of this function might directly write and compile a tex file.

**Value**

This function produces a directory and moves all the files of namesFiles to it, then it creates an html report that contains info about the optimisation process.

**Author(s)**

C. Terfve

**See Also**

`writeNetwork`, `writeScaffold`

**Examples**

tmpdir<-tempdir()
setwd(tmpdir)

# load data
data(CNOlistToy, package="CellNOptR")
data(ToyModel, package="CellNOptR")

# pre-process model (partial)
indicesToy<-indexFinder(CNOlistToy, ToyModel, verbose=TRUE)
ToyNCNOcutComp<-compressModel(ToyModel, indicesToy)
indicesToyNCNOcutComp<-indexFinder(CNOlistToy, ToyNCNOcutComp)
ToyNCNOcutCompExp<-expandGates(ToyNCNOcutComp)

# optimise
ToyFields4Sim<-prep4sim(ToyNCNOcutCompExp)
initBstring<-rep(1, length(ToyNCNOcutCompExp$reactID))
ToyT1opt<-gaBinaryT1(
  CNOlist=CNOlistToy,
  model=ToyNCNOcutCompExp,
  initBstring=initBstring,
  maxGens=2,
  popSize=5,
  verbose=TRUE)

# write report
namesFilesToy<-list(
dataPlot=NA,
evolFitT1=NA,
writeScaffold

Writes the scaffold network to a sif file (with attributes) and to a dot file

Description

This function writes a cytoscape SIF file for the scaffold network, with an associated edge attribute file that holds whether the edge is present at t1,t2 or not present at all and another associated edge attribute file that holds the weights of the edges. This function also writes a dot file that contains the same information (see writeDot for more information about the dot file conventions).

Usage

writeScaffold(modelComprExpanded, optimResT1, optimResT2, modelOriginal, CNOlist, tag=NULL)

Arguments

modelComprExpanded  The scaffold model (i.e. compressed and expanded)
optimResT1  The results of the optimisation process at t1
optimResT2  The results of the optimisation process at t2 (set this to NA if you have performed a one time point optimisation).
modelOriginal  The PKN model
CNOlist  The CNOlist on which the optimisation is based
tag  NULL or string; tells whether you want to prefix filenames with a tag (replaces the default behaviour).
Details

By scaffold network we mean the network that is used as a basis for optimisation (i.e. a compressed and expanded network), therefore no map back of the weights is necessary here.

The weights of the edges are computed as the mean across models within the relative tolerance limits, as output in the results from the optimisation $\text{stringsTol}$. Strings that are in $\text{stringsTol}$ are the ones that are within the relative tolerance limits around the best solution in the population across all generations of the optimisation.

If there is no time 2, then the argument optimResT2 should be = NA.

Value

This function does not return anything, it writes a sif file and 2 edge attributes files, and a dot file, in your working directory.

Author(s)

C.Terfve

See Also

writeNetwork, writeDot

Examples

tmpdir<-tempdir()
setwd(tmpdir)

#load the data
data(CNOlistToy,package="CellNOptR")
data(ToyModel,package="CellNOptR")

#pre-process the model (partial)
indicesToy<-indexFinder(CNOlistToy,ToyModel,verbose=TRUE)
ToyNCNOcutComp<-compressModel(ToyModel,indicesToy)
indicesToyNCNOcutComp<-indexFinder(CNOlistToy,ToyNCNOcutComp)
ToyNCNOcutCompExp<-expandGates(ToyNCNOcutComp)

#optimise

ToyFields4Sim<-prep4sim(ToyNCNOcutCompExp)
initBstring<-rep(1,length(ToyNCNOcutCompExp$reacID))
ToyT1opt<-gaBinaryT1(
CN0list=CNOlistToy,
model=ToyNCNOcutCompExp,
initBstring=initBstring,
maxGens=3,
popSize=5,
verbose=TRUE)

#write the network

writeScaffold(
modelOriginal=ToyModel,
writeSIF

Convert a model into a SIF format and save the result in a file.

Description

This function takes as input a model (as created by e.g., read from a SIF data set with readSIF function) and save it into a file.

Usage

writeSIF(model, filename, overwrite = FALSE)

Arguments

model the model
filename the filename
overwrite by default, do not overwrite a file.

Author(s)

T Cokelaer

Examples

tmpdir<-tempdir()
setwd(tmpdir)
cpfile<-dir(system.file("ToyModel",package="CellNOptR"),full=TRUE)
file.copy(from=cpfile,to=getwd(),overwrite=TRUE)
ToyModel<-readSIF(sifFile="ToyPNMMB.sif")
writeSIF(ToyModel, "ToyPNMMB_copy.sif")
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