Package 'dynafluxr'

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Type Package

Title Retrieve Reaction Rate Dynamics from Metabolite Concentration Time Courses

Version 1.0.1

Description Reaction rate dynamics can be retrieved from metabolite concentration time courses. User has to provide corresponding stoichiometric matrix but not a regulation model (Michaelis-Menten or similar).
Instead of solving an ordinary differential equation (ODE) system describing the evolution of concentrations,
we use B-splines to catch the concentration and rate dynamics then solve a least square problem on their coefficients with non-negativity (and optionally monotonicity) constraints.
Constraints can be also set on initial values of concentration.
The package 'dynafluxr' can be used as a library but also as an application with command line interface dynafluxr::cli(``-h'') or graphical user interface dynafluxr::gui().

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Encoding UTF-8

Depends bspline (>= 2.5.0), nlsic (>= 1.1.1)

Imports optparse, qpdf, arrApply, slam, gmresls (>= 0.2), shiny, shinyjs, shinyFiles

RoxygenNote 7.3.2

Suggests RUnit, knitr

VignetteBuilder knitr

NeedsCompilation no

Author Serguei Sokol [aut, cre]

Maintainer Serguei Sokol <sokol@insa-toulouse.fr>

Repository CRAN

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Contents

`cli` *Function to be called from shell command line*

Description

Function to be called from shell command line

Usage

```
cli(args = commandArgs(trailingOnly = TRUE))
```

Arguments

`args`	Character vector, command line parameters (default `commandArgs(trailingOnly=TRUE)`)

Details

run `cli("-h")` in R or `Rscript -e 'dynafluxr::cli()' -h` in shell to get a help page with available option description

Value

a list resulting from `fdyn()` call

See Also

fdyn

Examples

```
# from shell
# $ Rscript --vanilla -e 'dynafluxr::cli()' -m data_kinetics.tsv -s glycolysis.txt

# from R session
ddir=system.file("dataglyco", package="dynafluxr")
meas=file.path(ddir, "data.tsv")
sto=file.path(ddir, "network.txt")
res=cli(c("-m", meas, "-s", sto, "--skip", "24", "-o", ""))
tp=res$tp
np=length(tp)
tpp=res$tpp
```

```
# plot species
matplot(tpp, res$msp(tpp), type="l")
matpoints(tp, res$mf[,-1], pch=".", cex=0.5)
legend("topright", legend=colnames(bsppar(res$msp)$qw), lty=1:5, col=1:6, cex=0.75)
# plot rates
dev.new()
matplot(tpp, res$vsp(tpp), type="l")
# plot residuals
dev.new()
matplot(tpp, res$risp(tpp), type="l")
legend("topright", legend=colnames(bsppar(res$rsp)$qw), lty=1:5, col=1:6, cex=0.75)
```

`fdyn` *Retrieve flux dynamics from metabolic kinetics*

Description

Retrieve flux dynamics from metabolic kinetics

Usage

```
fdyn(
  mf,
  stofull,
  nsp = 4L,
  nki = 5L,
  lieq = NULL,
  monotone = 0,
  dls = FALSE,
  atomlen = NULL,
  npi = 300L,
  wsd = FALSE,
  nmsf = character(0L),
  sderr = NULL,
  tol = 1e-10,
  regular_grid = TRUE
)
```

Arguments

`mf`	Data-frame or matrix, specie kinetic measurements. Columns must be named with specie names and 'Time'.
`stofull`	Full stoichiometric matrix, `stofull[i,j]` means reaction 'j' produces specie 'i' with coeficient 'stofull[i,j]'. If `stofull[i,j] < 0`, the specie 'i' is consumed. Columns must be named with reaction names. Rows must be names with the species. "Full" in the name means that matrix includes even NA species.
`nsp`	Integer, polynomial order of B-spline to use for species (default 4)

nki	Integer, number of internal knots for B-splines (default 5)
lieq	List, equality constraints on species (default NULL, i.e. no equality constraint)
monotone	Numeric scalar or vector, 1=species are monotonically increasing; -1=monotonically decreasing; 0=no constraint. If vector, each value constraints (or not) a corresponding data column in mf ('Time' column is excluded from counting) (default 0, i.e. no monotonicity constraint)
dls	Logical scalar, if TRUE, indicates that differential least squares should be resolved instead of integral least squares. (default FALSE, i.e. ILS will be used)
atomlen	Numerical named vector, indicates what is label length of a given specie used a vector item name. If provided, results will contain `lsp` and `ilsp` fields which are a B-spline function representing atom balance over msp and isp splines. (default NULL, i.e. no atom balance will be provided)
npi	Integer scalar, indicates a number of plot intervals to produce smooth plots. (default 300)
wsd	Logical scalar, if TRUE, indicates that differential least squares should be resolved with residuals weighted by a factor of covariance matrix. (default FALSE, i.e. no weighting is used)
nmsf	Character vector, list of species for which scaling factor maust be estimated for –dls.
sderr	Numeric vector, use this SD of measured metabolites instead of automatically estimated. The name of each vector component is metabolite name, tha value is SD vale, e.g. `c(GLC=0.1)` (default NULL, i.e. SD are automatically estimated).
tol	Double scalar, tolerance for detecting singular matrices and solving linear systems
regular_grid	Logical scalar, use regular knot grid (default: TRUE)

Details

Each item in `lieq` corresponds to a specie and is a 2 column matrix (Time, Value). Each row of this matrix indicates what 'Value' must take corresponding specie at what 'Time'. Typically, it can be used to impose starting values at Time=0 for some species.
All specie fits are constraint to have values >= 0.

Value

List with following components:

mf: specie data frame used for fitting

tp: vector of time points for used measurements

tpp: vector of time points for plot (fine time resolution)

sto: stoichiometric matrix used for fitting

stofull: stoichiometric matrix before a possible NA elimination

stoinv: pseudo-inverse of sto

msp: measured specie spline function

vsp: estimated rates spline function

fsp: estimated total flux (S*v) spline function

dsp: first derivative of measured spline function

isp: integrated specie spline function

asp: atom balance over msp spline function

iasp: atom balance over isp spline function

vsp: flux spline function

dsp: measured specie first derivative spline function

rsp: residual `dM/dt - S%*%v` spline function

risp: integral residual `M - \u222bS%*%v dt` spline function

sdrate: matrix of SD values for flux B-spline coefficients, of size (`ncoef x nrate`)

chi2tab: data-frame with chi2-test results

sf: named scale factor vector

internal_knot_ref: number of internal knots used for estimation of var_ref

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`gui` *Launch graphical user interface in web browser*

Description

Launch graphical user interface in web browser

Usage

```
gui()
```

Value

no returned value

`txt2sto` *Translate plain text file with reactions to stoichiometric matrix*

Description

Translate plain text file with reactions to stoichiometric matrix

Usage

```
txt2sto(fn)
```

Arguments

`fn`	String, file name

Value

Matrix of size n_metab x n_reac

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