Package ‘fbar’

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Type Package
Title An Extensible Approach to Flux Balance Analysis
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Description A toolkit for Flux Balance Analysis and related metabolic modeling techniques. Functions are provided for: parsing models in tabular format, converting parsed metabolic models to input formats for common linear programming solvers, and evaluating and applying gene-protein-reaction mappings. In addition, there are wrappers to parse a model, select a solver, find the metabolic fluxes, and return the results applied to the original model. Compared to other packages in this field, this package puts a much heavier focus on providing reusable components that can be used in the design of new implementation of new techniques, in particular those that involve large parameter sweeps. For a background on the theory, see What is Flux Balance Analysis <doi:10.1038/nbt.1614>.
License GPL-3
BugReports https://github.com/maxconway/fbar/issues
Depends R (>= 3.3.0)
Imports assertthat, dplyr, magrittr, Matrix, purrr, rlang, ROI, ROI.plugin.ecos, stringr, tibble, tidyr
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decompose_metabolites

Decompose a metabolite table into the metabolite stub itself and the compartment it is in

Description

Decompose a metabolite table into the metabolite stub itself and the compartment it is in

Usage

decompose_metabolites(
  met_table,
  compartment_regex = "([\[A-Z0-9]+])|([a-zA-Z])"
)
ecoli_core

Arguments

met_table
A metabolite table, with one column, met

compartment_regex
Regular expression to identify compartments in model

Value

A metabolite table with the columns chemical and compartment

Examples

data(ecoli_core)
mod <- reactiontbl_to_expanded(ecoli_core)
decompose_metabolites(mod$mets)
recompose_metabolites(decompose_metabolites(mod$mets))

ecoli_core
A small E. coli model, created from a number of sources.

Description

A small E. coli model, created from a number of sources.

Usage

ecoli_core

Format

A data frame with 95 rows and 7 columns:

abbreviation an abbreviated reaction name, acts as the reaction id
lowbnd lower bound on the reaction rate
uppbnd upper bound on the reaction rate
obj_coef identifies a reaction (or reactions) for which the maximum possible rate should be found
equation reaction equation
officialName full reaction name
geneAssociation A boolean combination of genes which control the reaction
subsystem an indicator of reaction function

Source

expanded_to_glpk  Parse a long format metabolic model to a glpk model

Description

This function is deprecated. ROI.plugin.glpk is recommended instead.

Usage

expanded_to_glpk(reactions_expanded)

Arguments

reactions_expanded
A list of data frames as output by reactiontbl_to_expanded

Details

This parses the long format produced by reactiontbl_to_expanded to a glpk model.

To install the Rglpk package in Linux, run sudo apt-get install libglpk-dev in a terminal, and then run install.packages('Rglpk') in R.

The reaction_table must have columns:

• abbreviation,
• equation,
• uppbnd,
• lowbnd, and
• obj_coef.

Value

A list suitable for input to Rglpk

See Also

Other parsing_and_conversion: expanded_to_ROI(), expanded_to_gurobi(), reactiontbl_to_expanded(), reactiontbl_to_gurobi()
expanded_to_gurobi

Parse a long format metabolic model to a Gurobi model

Description

This function is deprecated. github.com/Fi0Sch/ROI.plugin.gurobi is recommended instead.

Usage

expanded_to_gurobi(reactions_expanded)

Arguments

reactions_expanded
A list of data frames as output by expand_reactions

Details

Used as the second half of reactiontbl_to_gurobi, this parses the long format produced by reactiontbl_to_expanded to a Gurobi model

For installation instructions for Gurobi, refer to the Gurobi website: https://www.gurobi.com/.

The reaction_table must have columns:

- abbreviation,
- equation,
- uppbnd,
- lowbnd, and
- obj_coef.

Value

A list suitable for input to Gurobi.

See Also

Other parsing_and_conversion: expanded_to_ROI(), expanded_to_glpk(), reactiontbl_to_expanded(), reactiontbl_to_gurobi()
expanded_to_reactiontbl

(Convert intermediate expanded format back to a reaction table)

Description

Useful for saving a new or edited model.

Usage

expanded_to_reactiontbl(expanded)

Arguments

expanded  A list of data frames:
  • rxns, which has one row per reaction,
  • mets, which has one row for each metabolite, and
  • stoich, which has one row for each time a metabolite appears in a reaction.

Value

A data frame describing the metabolic model.

expanded_to_ROI

(Parse a long format metabolic model to an ROI model)

Description

This parses the long format produced by reactiontbl_to_expanded to an ROI model.

Usage

expanded_to_ROI(reactions_expanded)

Arguments

reactions_expanded  A list of data frames as output by reactiontbl_to_expanded
To solve models using ROI, you will need a solver plugin for ROI. Probably the easiest one to install is ROI.plugin.glpk. To install this in Linux, run `sudo apt-get install libglpk-dev` in a terminal, and then run `install.packages('ROI.plugin.glpk')` in R.

The `reaction_table` must have columns:

- abbreviation,
- equation,
- uppbnd,
- lowbnd, and
- obj_coef.

**Value**

A list suitable for input to ROI.

**See Also**

Other parsing_and_conversion: `expanded_to_glpk()`, `expanded_to_gurobi()`, `reactiontbl_to_expanded()`, `reactiontbl_to_gurobi()`

**Examples**

```r
## Not run:
data(ecoli_core)
library(dplyr)
try(library(ROI.plugin.ecos)) # make a solver available to ROI

roi_model <- ecoli_core %>%
  reactiontbl_to_expanded %>%
  expanded_to_ROI

if(length(ROI::ROI_applicable_solvers(roi_model))>=1){
  roi_result <- ROI::ROI_solve(roi_model)

  ecoli_core_with_flux <- ecoli_core %>%
    mutate(flux = roi_result[['solution']])
}
```

## End(Not run)
**fbar:** Flux Balance Analysis in R with a tidy data approach

**Description**

fbar is a simple, easy to use Flux Balance Analysis package with a tidy data approach. Just data frames and the occasional list, no new classes to learn. The focus is on simplicity and speed. Models are expected as a flat table, and results can be simply appended to the table. This makes this package very suitable for use in pipelines with pre- and post- processing of models and results, so that it works well as a backbone for customized methods. Loading, parsing and evaluating a model takes around 0.1s, which, together with the straightforward data structures used, makes this library very suitable for large parameter sweeps.

**Details**

For a list of functions in the package, see vignette('Introduction','fbar')

---

**find_fluxes_df**

*Given a metabolic model as a data frame, return a new data frame with fluxes*

**Description**

Given a metabolic model as a data frame, return a new data frame with fluxes

**Usage**

`find_fluxes_df(reaction_table, do_minimization = FALSE)`

**Arguments**

- `reaction_table`: a data frame representing the metabolic model
- `do_minimization`: toggle to uniformly minimize all non-objective fluxes after finding the objective

**Details**

This function uses ROI, so to solve models, you will need a solver plugin for ROI. Probably the easiest one to install is ROI.plugin.glpk. To install this in Linux, run `sudo apt-get install libglpk-dev` in a terminal, and then run `install.packages('ROI.plugin.glpk')` in R.

**Value**

The input data frame with a new numeric column, "flux".
find_flux_variability_df

See Also
find_fluxes_vector

Examples

## Not run:
data(ecoli_core)
ecoli_core_with_flux <- find_fluxes_df(ecoli_core)
## End(Not run)

find_flux_variability_df

Given a metabolic model as a data frame, return a new data frame with fluxes and variability

Description

This function calculates fluxes folds times with shuffled versions of the metabolic model. This is designed to detect and quantify underdetermined fluxes.

Usage

find_flux_variability_df(reaction_table, folds = 10, do_minimization = TRUE)

Arguments

reaction_table  a data frame representing the metabolic model
folds  number of times to calculate fluxes
do_minimization  toggle to uniformly minimize all non-objective fluxes after finding the objective

Details

This function uses ROI, so to solve models, you will need a solver plugin for ROI. Probably the easiest one to install is ROI.plugin.glpk. To install this in Linux, run `sudo apt-get install libglpk-dev` in a terminal, and then run `install.packages('ROI.plugin.glpk')` in R.

Value

reaction_table with two added columns: sd (the standard deviation of fluxes found) and flux (a typical flux) from this distribution
gene_associate

Apply gene expressions to reaction table

Description
A convenience function that uses gene_eval and a custom function to apply new upper and lower bounds.

Usage
gene_associate(
  reaction_table,
  gene_table,
  expression_flux_function = function(x) {
    (1 + log(x)/stats::sd(x)^2)^sign(x - 1)
  }
)

Arguments
  reaction_table  A data frame describing the metabolic model.
  gene_table      A data frame showing gene presence
  expression_flux_function
                  a function to convert from gene set expression to flux

Value
the reaction_table, with a new column, present, and altered upper and lower bounds

Warning
This function relies on gene_eval, which uses eval to evaluate gene expression sets. This gives flexibility, but means that malicious code in the gene_sets argument could get evaluated. gene_sets is evaluated in a restricted environment, but there might be a way around this, so you might want to check for anything suspicious in this argument manually. For more information, read the code.

See Also
gene_eval

Examples
data(iJO1366)
library(dplyr)

gene_table = tibble(name = iJO1366$geneAssociation %>%
  stringr::str_split('and|or|\s|\(|\)') %>%
  purrr::flatten_chr() %>%
  unique,
gene_eval

Function to estimate the expression levels of gene sets

description
Function to estimate the expression levels of gene sets

Usage

gene_eval(gene_sets, genes, presences)

Arguments

gene_sets A list of gene set strings: names of genes punctuated with & and brackets.
genes A list of gene names
presences A list of gene presences, the same length as genes

Value

A vector the same length as gene_sets, with the calculated combined gene expression levels.

This function evaluates the gene sets in the context of the gene presences. It can take booleans, or
numbers, in which case it associates & with finding the minimum, and | with finding the maximum.

Warning

This function uses eval to evaluate gene expression sets. This gives flexibility, but means that
malicious code in the gene_sets argument could get evaluated. gene_sets is evaluated in a re-
stricted environment, but there might be a way around this, so you might want to check for anything
suspicious in this argument manually. For more information, read the code.

See Also

gene_associate
**get_BiGG**  
*Download a model from a BiGG json file*

**Description**
Download a model from a BiGG json file

**Usage**
get_BiGG(address)

**Arguments**
- address: An address to download from

**Value**
A model in expanded format

---

**iJO1366**  
*A full size E. coli model.*

**Description**
A full size E. coli model.

**Usage**
iJO1366

**Format**
A data frame with 2,583 rows and 10 columns:
- **abbreviation**: an abbreviated reaction name, acts as the reaction id
- **lowbnd**: lower bound on the reaction rate
- **uppbnd**: upper bound on the reaction rate
- **obj_coef**: identifies a reaction (or reactions) for which the maximum possible rate should be found
- **equation**: reaction equation
- **officialName**: full reaction name
- **geneAssociation**: A boolean combination of genes which control the reaction
- **subsystem**: an indicator of reaction function

**Source**
### nutrient_types

A subset of exchange reactions annotated to indicate typical availability

#### Description
A subset of exchange reactions annotated to indicate typical availability

#### Usage
nutrient_types

#### Format
A data frame with 25 rows and 2 columns:

- **abbreviation**: an exchange reaction id
- **nutrient_type**: the nutrient availability, one of 'micro', 'macro' or 'substrate'

### parse_met_list

Internal function: Expand half reaction equations into a long form

#### Description
Internal function: Expand half reaction equations into a long form

#### Usage
parse_met_list(mets)

#### Arguments
- **mets**: Character vector of halves of reaction equations.

#### Value
A data frame with columns:

- **stoich**: the stoichiometric coefficient
- **met**: the metabolite
reactiontbl_toExpanded

Parse a reaction table to an intermediate, long format

Description

The long format can also be suitable for manipulating equations.

Usage

reactiontbl_toExpanded(reaction_table, regex_arrow = "<?[-=]+>")

Arguments

reaction_table  A data frame describing the metabolic model.
regex_arrow    Regular expression for the arrow splitting sides of the reaction equation.

Details

The reaction_table must have columns:

• abbreviation,
• equation,
• uppbnd,
• lowbnd, and
• obj_coef.

Value

A list of data frames:

• rxns, which has one row per reaction,
• mets, which has one row for each metabolite, and
• stoich, which has one row for each time a metabolite appears in a reaction.

See Also

Other parsing_and_conversion: expanded_to_ROI(), expanded_to_glpk(), expanded_to_gurobi(), reactiontbl_to_gurobi()
Examples

```r
## Not run:
data(ecoli_core)
library(dplyr)
try(library(ROI.plugin.ecos)) # make a solver available to ROI

roi_model <- ecoli_core %>%
  reactiontbl_to_expanded %>%
  expanded_to_ROI

if(length(ROI::ROI_applicable_solvers(roi_model))>=1){
  roi_result <- ROI::ROI_solve(roi_model)

  ecoli_core_with_flux <- ecoli_core %>%
    mutate(flux = roi_result[['solution']])
}
## End(Not run)

---

reactiontbl_to_gurobi  Parse reaction table to Gurobi format

Description

This function is deprecated. github.com/Fl0Sch/ROI.plugin.gurobi is recommended instead.

Usage

`reactiontbl_to_gurobi(reaction_table, regex_arrow = "<\?[\-=]+")"

Arguments

reaction_table  A data frame describing the metabolic model.
regex_arrow      Regular expression for the arrow splitting sides of the reaction equation.

Details

Parses a reaction table to give a list in Gurobi’s input format. This function is a shorthand for `reactiontbl_to_expanded` followed by `expanded_to_gurobi`.

The `reaction_table` must have columns:

- abbreviation,
- equation,
- uppbnd,
- lowbnd, and
- obj_coef.
Value
A list suitable for input to Gurobi.

See Also
Other parsing and conversion: expanded_to_ROI(), expanded_to_glpk(), expanded_to_gurobi(), reactiontbl_to_expanded()

recompose_metabolites  Merge metabolite stub and compartment to form an id

Description
Merge metabolite stub and compartment to form an id

Usage
recompose_metabolites(
  expanded_metabolites,
  before_signifier = "_",
  after_signifier = ""
)

Arguments
expanded_metabolites
  a metabolite table as created by decompose_metabolites
before_signifier
  a string that is inserted before the compartment identifier
after_signifier
  a string that is inserted after the compartment identifier

Value
A merged metabolite table with one column, met

Examples
data(ecoli_core)
mod <- reactiontbl_to_expanded(ecoli_core)
decompose_metabolites(mod$mets)
recompose_metabolites(decompose_metabolites(mod$mets))
### split_on_arrow

**Description**

Internal function: Splitting reaction equation into substrate and product

**Usage**

```r
split_on_arrow(equations, regex_arrow = "<?[-=]+>")
```

**Arguments**

- `equations` Character vector of reaction equations.
- `regex_arrow` Regular expression for the arrow splitting sides of the reaction equation.

**Value**

A data frame, with columns:
- `reversible` boolean, is reaction reversible
- `before` the left hand side of the reaction string
- `after` the right hand side of the reaction string

---

### validate_expanded

**Description**

Validate an expanded model

**Usage**

```r
validate_expanded(reactions_expanded)
```

**Arguments**

- `reactions_expanded` the expanded model to check

**Value**

`TRUE`
Index

* datasets
  ecoli_core, 3
  iJO1366, 12
  nutrient_types, 13

* parsing_and_conversion
  expanded_to_glpk, 4
  expanded_to_gurobi, 5
  expanded_to_ROI, 6
  reactiontbl_to_expanded, 14
  reactiontbl_to_gurobi, 15

decompose_metabolites, 2, 16

ecoli_core, 3
  eval, 10, 11
  expanded_to_glpk, 4, 5, 7, 14, 16
  expanded_to_gurobi, 4, 5, 7, 14–16
  expanded_to_reactiontbl, 6
  expanded_to_ROI, 4, 5, 6, 14, 16

fbar, 8
  find_flux_variability_df, 9
  find_fluxes_df, 8

gene_associate, 10
  gene_eval, 10, 11
  get_BiGG, 12

iJO1366, 12

nutrient_types, 13

parse_met_list, 13

reactiontbl_to_expanded, 4, 5, 7, 14, 15, 16

reactiontbl_to_gurobi, 4, 5, 7, 14, 15

recompose_metabolites, 16

split_on_arrow, 17

validate_expanded, 17