

Package: METAFLEX (via r-universe)

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Title High-Performance Metabolic Flux Analysis from Bulk and Single-Cell RNA-seq Data

Version 2.2.0

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Description A performance-optimized implementation of METAFlex for characterizing cellular metabolism from bulk and single-cell RNA-sequencing data. Uses genome-scale metabolic modeling with Human-GEM to derive 13,082 metabolic fluxes through flux balance analysis (FBA). Features parallel computing, Rcpp acceleration, and optimized algorithms for 10-20x faster computation.

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URL <https://zaoqu-liu.github.io/METAFlex/>,
<https://github.com/Zaoqu-Liu/METAFlex>

BugReports <https://github.com/Zaoqu-Liu/METAFlex/issues>

Encoding UTF-8

LazyData true

Roxygen list(markdown = TRUE)

RoxygenNote 7.3.3

Depends R (>= 3.6.0)

Imports stringr, osqp, stringi, Seurat (>= 4.0.0), dplyr, Matrix, parallel, foreach, doParallel, utils, Rcpp

Suggests rmarkdown, knitr, testthat (>= 3.0.0)

LinkingTo Rcpp

VignetteBuilder knitr

Config/testthat/edition 3

Config/pak/sysreqs cmake libglpk-dev make libicu-dev libpng-dev libuv1-dev libxml2-dev libssl-dev python3 zlib1g-dev

Repository <https://zaoqu-liu.r-universe.dev>
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bulk_test_example	<i>Bulk test example</i>
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Description

Bulk test example

Usage

```
bulk_test_example
```

Format

A data frame with 58581 rows and 5 variables

Examples

```
data(bulk_test_example)
```

calculate_avg_exp *Calculate bootstrap mean expression for single cell data*

Description

Calculate bootstrap mean expression for single cell data

Usage

```
calculate_avg_exp(myseurat, myident, n_bootstrap, seed)
```

Arguments

myseurat	Seurat object. METAFLUX will calculate on "data" slot
myident	Seurat idents for grouping. This will be a character string indicating the grouping of the seurat object
n_bootstrap	number of bootstrap
seed	random seed

Value

mean expression data

calculate_reaction_score *Calculate metabolic reaction scores (MRAS) for 13082 reactions*

Description

Calculate metabolic reaction scores (MRAS) for 13082 reactions

Usage

```
calculate_reaction_score(data)
```

Arguments

data	gene expression data. 1. The gene expression matrix should be gene by sample matrix where row names are human gene names (gene symbols), and column names should be sample names. Please note that METAFLUX does not support other gene IDs. 2. The input gene expression matrix should be normalized (e.g., log-transformed, etc.) before using METAFLUX. METAFLUX will not perform any normalization on expression data. 3. Gene expression data cannot have negative values.
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cell_medium	<i>This file contains the hams medium nutrients information</i>
-------------	---

Description

This default file indicates the nutrients available in the medium. There are total 44 metabolites available. This file can be changed depending on users. We will allow users to define the medium profile based on their knowledge.

Usage

```
cell_medium
```

Format

A data frame with 44 rows and 2 variables:

metabolite stands for name of nutrients available in the medium.

reaction_name V2 stands for reaction ID of corresponding nutrients

Examples

```
data(cell_medium)
```

compute_flux	<i>Final optimization step for flux calculation</i>
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Description

Final optimization step for flux calculation

Usage

```
compute_flux(mras, medium)
```

Arguments

mras	metabolic reaction activity scores
medium	input medium file which indicates the nutrients available in the medium. We provide 2 general mediums if you have no prior knowledge about your medium: cell line medium and human blood medium if prior knowledge is not available. Please see tutorial for more details.

Value

Calculated fluxes

compute_sc_flux	<i>Single-Cell RNA-seq Metabolic Flux Calculation</i>
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Description

Computes metabolic fluxes for single-cell RNA-seq data using community modeling.

Usage

```
compute_sc_flux(
  num_cell,
  fraction,
  fluxscore,
  medium,
  parallel = TRUE,
  n_cores = NULL,
  use_cpp = TRUE
)
```

Arguments

num_cell	Integer. Number of cell types or clusters.
fraction	Numeric vector. Fraction of each cell type (must sum to 1).
fluxscore	Matrix. Metabolic reaction activity scores (MRAS) from bootstrap sampling.
medium	Data frame. Medium profile specifying available nutrients.
parallel	Logical. Use parallel computing? (default: TRUE)
n_cores	Integer. Number of CPU cores (default: NULL = auto-detect, max 8)
use_cpp	Logical. Use C++ optimization? (default: TRUE)

Value

Data frame of metabolic fluxes for single-cell community model.

human_blood	<i>This file contains the hams medium nutrients information in human blood</i>
-------------	--

Description

This default file indicates the nutrients available in the medium. There are total 44 metabolites available. This file can be changed depending on users. We will allow users to define the medium profile based on their knowledge.

Usage

```
human_blood
```

Format

A data frame with 44 rows and 2 variables:

metabolite stands for name of nutrients available in the human blood.

reaction_name stands for reaction ID of corresponding nutrients

Examples

```
data(human_blood)
```

human_gem	<i>Human-GEM Metabolic Model Data</i>
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Description

Human genome-scale metabolic model (Human-GEM) containing reaction, gene, and pathway information for metabolic flux analysis.

Usage

```
human_gem
```

Format

A data frame with 13,082 rows (reactions) and 16 variables:

Row number

ID Reaction ID

NAME Reaction name

EQUATION Stoichiometric equation

EC-NUMBER Enzyme Commission number

GENE ASSOCIATION Gene-protein-reaction rule

LOWER BOUND Lower flux bound

UPPER BOUND Upper flux bound

OBJECTIVE Objective function coefficient (1 for biomass)

COMPARTMENT Cellular compartment

MIRIAM MIRIAM annotations

SUBSYSTEM Metabolic pathway/subsystem

REPLACEMENT ID Alternative reaction ID

NOTE Additional notes

REFERENCE Literature references

CONFIDENCE SCORE Reaction confidence score

Source

<https://github.com/SysBioChalmers/Human-GEM>

Examples

```
data(human_gem)
head(human_gem)
```

nutrient_lookup_files *1648 exchange reactions:mathematical representation of uptake/secrete metabolites into the extracellular space*

Description

1648 exchange reactions:mathematical representation of uptake/secrete metabolites into the extracellular space

Usage

```
nutrient_lookup_files
```

Format

1648 rows

Examples

```
data("nutrient_lookup_files")
```

sc_test_example *single cell test seurat object example*

Description

single cell test seurat object example

Usage

```
sc_test_example
```

Format

A toy example containing 350 cells(Tumor and T cells)

Examples

```
data(sc_test_example)
```

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