

Package ‘RCOMET’

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Title Package for context-specific optimization of EMT trajectories

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Description COMET is a computational framework for inferring EMT trajectories from time-course single cell RNA sequencing data.

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Encoding UTF-8

Roxygen list(markdown = TRUE)

RoxygenNote 7.2.3

Suggests knitr, rmarkdown, devtools, diagram, ggplot2, ggpubr, grid, gridExtra, plotly, tidyr, tidyverse, Rmagic

VignetteBuilder knitr

Imports Seurat,

umap,
dtw,
pracma,
dplyr,
readxl,
reshape2,
data.table,
expm,
Rmisc,
stats

Depends phateR

R topics documented:

calculate_conf_intervals	2
DTW_calculate	2
find.min.alpha	3
find.optimal.cutoff	3
fit.all.data	4
fit.CTMC	4
generate_pipeline_files	5
KS.label.me	5

run.CTMC	6
run_pipeline	6
start_pipeline	7
transition_matrix	7

Index	8
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calculate_conf_intervals

This function calculates confidence intervals for every sample over 10 runs

Description

This function calculates confidence intervals for every sample over 10 runs

Usage

```
calculate_conf_intervals(data.inputs)
```

Arguments

data.inputs the input datasheet stored in a csv file in the tables dir

Value

nothing, saves results within the Confidence_Interval_Calculations dir

DTW_calculate

This function calculates the DTW distance bewteen the inferred trajectories for every cutoff and the flow cytometry data

Description

This function calculates the DTW distance bewteen the inferred trajectories for every cutoff and the flow cytometry data

Usage

```
DTW_calculate(data.inputs, MET.range)
```

Arguments

data.inputs the input datasheet stored in a csv file in the tables dir
 MET.range range of time for MET to take place

Value

nothing, saves the matrix in the DTW_Matrix dir

find.min.alpha	<i>This function finds the mse_total given a certain alpha</i>
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Description

This function finds the mse_total given a certain alpha

Usage

```
find.min.alpha(
  alpha,
  E_cad,
  hybrid,
  ZEB,
  M_sc,
  Mu_sc,
  eq,
  ref_eq_day,
  timepoints
)
```

Arguments

alpha	parameter alpha
E_cad	Epithelial percentage, just named E_cad
hybrid	hybrid percentage
ZEB	Mesenchymal percentage, just named ZEB
M_sc	ratio of M/E at steady state
Mu_sc	ratio of H/E at steady state
eq	what timepoint to start
ref_eq_day	steady state timepoint
timepoints	total timepoints

Value

mse_total

find.optimal.cutoff	<i>Find the optimal cutoff Finds the best number of highly variable EMT genes</i>
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Description

Find the optimal cutoff Finds the best number of highly variable EMT genes

Usage

```
find.optimal.cutoff(data.input)
```

Arguments

data.input input data to use

Value

optimal cutoff of highly variable genes

fit.all.data	<i>This function fits optimal CTMC trajectories to timecourse data</i>
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Description

This function fits optimal CTMC trajectories to timecourse data

Usage

```
fit.all.data(data.inputs, MET.range)
```

Arguments

data.inputs the input datasheet stored in a csv file in the tables dir
 MET.range range of time for MET to take place

Value

the final dataframe with the optimal trajectories fitted to data

fit.CTMC	<i>This function optimally fits 3 CTMC models to data (1st phase, 2nd phase, MET range)</i>
----------	---

Description

This function optimally fits 3 CTMC models to data (1st phase, 2nd phase, MET range)

Usage

```
fit.CTMC(data.input, MET.range, opt.cutoff)
```

Arguments

data.input input data to use
 MET.range range where MET takes place
 opt.cutoff optimal cutoff of highly variable genes

Value

final trajectories, lambda_E, mu, and lambda_M respectively

generate_pipeline_files

This function is to be ran for all cutoffs, purpose is to find the optimal number of EMT genes to minimize the DTW distance between the flow cytometry trajectories and data

Description

This function is to be ran for all cutoffs, purpose is to find the optimal number of EMT genes to minimize the DTW distance between the flow cytometry trajectories and data

Usage

```
generate_pipeline_files(data.inputs, tables.dir, input.data.dir)
```

Arguments

data.inputs the input datasheet stored in a csv file in the tables dir
 tables.dir directory with a csv file that had the address for the data and metadata
 input.data.dir this is the directory where the input file should be saved in

Value

does not return, saves the files in the COMET_populated_files dir

KS.label.me

This function perform Kolmogorov Smirnov scoring on data, credit given to Priyanka Chakraborty as the code was adapted from her work and modified

Description

This function perform Kolmogorov Smirnov scoring on data, credit given to Priyanka Chakraborty as the code was adapted from her work and modified

Usage

```
KS.label.me(exp.mat, genes, topgenes)
```

Arguments

exp.mat gene expression matrix
 genes genes
 topgenes receives top 200 highly variable genes for scoring

Value

KS score

run.CTMC	<i>This function generates trajectories for a CTMC model given parameters</i>
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Description

This function generates trajectories for a CTMC model given parameters

Usage

```
run.CTMC(alph_fun, time.range, M_sc_fun, Mu_sc_fun, p0_fun)
```

Arguments

alph_fun	alpha parameter used in function
time.range	specific timerange to generate trajectory
M_sc_fun	ratio of M/E at steady state
Mu_sc_fun	ratio of H/E at steady state
p0_fun	initial state vector

Value

trajectories along with the resulting p vector

run_pipeline	<i>This function runs the data driven pipeline for inferring trajectories</i>
--------------	---

Description

This function runs the data driven pipeline for inferring trajectories

Usage

```
run_pipeline(data.inputs, tables.dir, input.data.dir, cutoff)
```

Arguments

data.inputs	the input datasheet stored in a csv file in the tables dir
tables.dir	directory with a csv file that had the address for the data and metadata
input.data.dir	this is the directory where the input file should be saved in
cutoff	of highly variable EMT genes to be considered

Value

the inferred trajectories, also saves them within the COMET_populated_files directory

start_pipeline	<i>Read necessary files and parameters for pipeline to run This function reads all the necessary files to run this pipeline</i>
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Description

Read necessary files and parameters for pipeline to run This function reads all the necessary files to run this pipeline

Usage

```
start_pipeline(tables.dir, input.data.dir)
```

Arguments

tables.dir directory with a csv file that had the address for the data and metadata
input.data.dir this is the directory where the input file should be saved in

Value

nothing, stores necessary parameters for the model in global variables

transition_matrix	<i>This function finds the transition matrix given the parameters for the generator matrix</i>
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Description

This function finds the transition matrix given the parameters for the generator matrix

Usage

```
transition_matrix(lambda_E, lambda_M, mu_E, mu_M, t)
```

Arguments

lambda_E Rate of transition from H to E
lambda_M Rate of transition from H to M
mu_E Rate of transition from E to H
mu_M Rate of transition from M to H
t time

Value

the probability transition matrix

Index

`calculate_conf_intervals`, [2](#)

`DTW_calculate`, [2](#)

`find.min.alpha`, [3](#)

`find.optimal.cutoff`, [3](#)

`fit.all.data`, [4](#)

`fit.CTMC`, [4](#)

`generate_pipeline_files`, [5](#)

`KS.label.me`, [5](#)

`run.CTMC`, [6](#)

`run_pipeline`, [6](#)

`start_pipeline`, [7](#)

`transition_matrix`, [7](#)