# Package 'COMET'

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Title COMET	
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<b>Description</b> COMET is a computational framework for inferring EMT trajectories from time-course single cell RNA sequencing data.	
License MIT	
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2 DTW\_calculate

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 3

#### **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

Mu\_sc ratio of H/E at steady star eq what timepoint to start ref\_eq\_day steady state timepoint timepoints total timepoints

#### Value

 $mse\_total$ 

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

#### **Description**

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

# Usage

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

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# **Arguments**

data.input input data to use

#### Value

optimal cutoff of highly variable genes

fit.all.data

This function fits optimal CTMC trajectories to timecourse data

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

phase, MET range)

# 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

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

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# 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

top200 receives top 200 highly variable genes for scoring

# Value

KS score

6 run\_pipeline

run.CTMC	This function generates trajectories for a CTMC model given param-
	eters

#### **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 This function runs the data driven pipeline for inferring trajectories

# 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

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

#### **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 This function finds the transition matrix given the parameters for the generator matrix	he
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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

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