

# Package ‘scMultiSim’

December 10, 2025

**Title** Simulation of Multi-Modality Single Cell Data Guided By Gene  
Regulatory Networks and Cell-Cell Interactions

**Version** 1.7.0

## Description

scMultiSim simulates paired single cell RNA-seq, single cell ATAC-seq and RNA velocity data, while incorporating mechanisms of gene regulatory networks, chromatin accessibility and cell-cell interactions. It allows users to tune various parameters controlling the amount of each biological factor, variation of gene-expression levels, the influence of chromatin accessibility on RNA sequence data, and so on. It can be used to benchmark various computational methods for single cell multi-omics data, and to assist in experimental design of wet-lab experiments.

**License** Artistic-2.0

**Encoding** UTF-8

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|                              |                                                                                               |
|------------------------------|-----------------------------------------------------------------------------------------------|
| <code>.amplifyOneCell</code> | <i>This function simulates the amplification, library prep, and the sequencing processes.</i> |
|------------------------------|-----------------------------------------------------------------------------------------------|

---

## Description

This function simulates the amplification, library prep, and the sequencing processes.

## Usage

```
.amplifyOneCell(  
  true_counts_1cell,  
  protocol,  
  rate_2cap,  
  gene_len,  
  amp_bias,  
  rate_2PCR,  
  nPCR1,  
  nPCR2,  
  LinearAmp,  
  LinearAmp_coef,  
  N_molecules_SEQ  
)
```

## Arguments

|                                |                                                                                   |
|--------------------------------|-----------------------------------------------------------------------------------|
| <code>true_counts_1cell</code> | the true transcript counts for one cell (one vector)                              |
| <code>protocol</code>          | a string, can be "nonUMI" or "UMI"                                                |
| <code>rate_2cap</code>         | the capture efficiency for this cell                                              |
| <code>gene_len</code>          | gene lengths for the genes/transcripts, sampled from real human transcript length |
| <code>amp_bias</code>          | amplification bias for each gene, a vector of length ngenes                       |
| <code>rate_2PCR</code>         | PCR efficiency, usually very high                                                 |

|                 |                                                                                                |
|-----------------|------------------------------------------------------------------------------------------------|
| nPCR1           | the number of PCR cycles                                                                       |
| nPCR2           | the number of PCR cycles                                                                       |
| LinearAmp       | if linear amplification is used for pre-amplification step, default is FALSE                   |
| LinearAmp_coef  | the coefficient of linear amplification, that is, how many times each molecule is amplified by |
| N_molecules_SEQ | number of molecules sent for sequencing; sequencing depth                                      |

**Value**

read counts (if protocol="nonUMI") or UMI counts (if protocol="UMI")

---

|                    |                                  |
|--------------------|----------------------------------|
| <i>.calAmpBias</i> | <i>Simulate technical biases</i> |
|--------------------|----------------------------------|

---

**Description**

Simulate technical biases

**Usage**

```
.calAmpBias(lenslope, nbins, gene_len, amp_bias_limit)
```

**Arguments**

|                |                                                                                                             |
|----------------|-------------------------------------------------------------------------------------------------------------|
| lenslope       | amount of length bias. This value should be less than $2 * \text{amp\_bias\_limit}[2] / (\text{nbins} - 1)$ |
| nbins          | number of bins for gene length                                                                              |
| gene_len       | transcript length of each gene                                                                              |
| amp_bias_limit | range of amplification bias for each gene, a vector of length ngenes                                        |

**Value**

a vector

---

|                             |                                                                                  |
|-----------------------------|----------------------------------------------------------------------------------|
| <code>.continuousCIF</code> | <i>Generates cifs for cells sampled along the trajectory of cell development</i> |
|-----------------------------|----------------------------------------------------------------------------------|

---

**Description**

Generates cifs for cells sampled along the trajectory of cell development

**Usage**

```
.continuousCIF(  
  seed,  
  N,  
  options,  
  ncell_key = "cell",  
  is_spatial = FALSE,  
  spatial_params = NULL,  
  .plot = FALSE,  
  .plot.name = "cont_cif.pdf"  
)
```

**Arguments**

|                             |                                      |
|-----------------------------|--------------------------------------|
| <code>seed</code>           | random seed                          |
| <code>N</code>              | the number list                      |
| <code>options</code>        | the option list                      |
| <code>ncell_key</code>      | the key for the number of cells in N |
| <code>is_spatial</code>     | return a list of cifs for spatial    |
| <code>spatial_params</code> | the spatial parameters               |
| <code>.plot</code>          | save the CIF plot                    |
| <code>.plot.name</code>     | plot name                            |

**Value**

a list containing the cif and meta data

---

|                                 |                                                                                              |
|---------------------------------|----------------------------------------------------------------------------------------------|
| <code>.divideBatchesImpl</code> | <i>Divide the observed counts into multiple batches by adding batch effect to each batch</i> |
|---------------------------------|----------------------------------------------------------------------------------------------|

---

### Description

Divide the observed counts into multiple batches by adding batch effect to each batch

### Usage

```
.divideBatchesImpl(
  counts,
  meta_cell,
  nbatch,
  batch_effect_size = 1,
  randseed = 0
)
```

### Arguments

|                                |                                                                                                            |
|--------------------------------|------------------------------------------------------------------------------------------------------------|
| <code>counts</code>            | gene cell matrix                                                                                           |
| <code>meta_cell</code>         | the meta information related to cells, will be combined with technical cell level information and returned |
| <code>nbatch</code>            | number of batches                                                                                          |
| <code>batch_effect_size</code> | amount of batch effects. Larger values result in bigger differences between batches. Default is 1.         |
| <code>randseed</code>          | random seed                                                                                                |

### Value

a list with two elements: counts and meta\_cell

---

|                              |                                                                                                            |
|------------------------------|------------------------------------------------------------------------------------------------------------|
| <code>.expandToBinary</code> | <i>expand transcript counts to a vector of binaries of the same length of as the number of transcripts</i> |
|------------------------------|------------------------------------------------------------------------------------------------------------|

---

### Description

expand transcript counts to a vector of binaries of the same length of as the number of transcripts

### Usage

```
.expandToBinary(true_counts_1cell)
```

### Arguments

true\_counts\_1cell  
number of transcript in one cell

### Value

a list of two vectors, the first vector is a vector of 1s, the second vector is the index of transcripts

---

.getCountCorrMatrix      *This function finds the correlation between every pair of genes*

---

### Description

This function finds the correlation between every pair of genes

### Usage

```
.getCountCorrMatrix(counts)
```

### Arguments

counts                  rna seq counts

### Value

the correlation matrix

---

.getParams                  *Get Kineic Parameters for all cells and genes*

---

### Description

Get Kineic Parameters for all cells and genes

### Usage

```
.getParams(seed, sim, sp_cell_i = NULL, sp_path_i = NULL)
```

### Arguments

seed                  random seed  
sim                  the simulation environment  
sp\_cell\_i              spatial cell index  
sp\_path\_i              the pre-sampled path along the tree for this cell

### Value

the kinetic parameters

---

|                     |                                                                   |
|---------------------|-------------------------------------------------------------------|
| .normalizeGRNParams | <i>Rename the original gene IDs in the GRN table to integers.</i> |
|---------------------|-------------------------------------------------------------------|

---

**Description**

Rename the original gene IDs in the GRN table to integers.

**Usage**

```
.normalizeGRNParams(params)
```

**Arguments**

params                      GRN parameters.

**Value**

list

---

|             |                                                  |
|-------------|--------------------------------------------------|
| .rnormTrunc | <i>sample from truncated normal distribution</i> |
|-------------|--------------------------------------------------|

---

**Description**

sample from truncated normal distribution

**Usage**

```
.rnormTrunc(n, mean, sd, a, b)
```

**Arguments**

n                      number of values to create  
mean                   mean of the normal distribution  
sd                      standard deviation of the normal distribution  
a                       the minimum value allowed  
b                       the maximum value allowed

**Value**

a vector of length n

---

|                |                                              |
|----------------|----------------------------------------------|
| add_expr_noise | <i>Add experimental noise to true counts</i> |
|----------------|----------------------------------------------|

---

**Description**

Add experimental noise to true counts

**Usage**

```
add_expr_noise(results, ...)
```

**Arguments**

|         |                                                                                                                                                                                                                                  |
|---------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| results | The scMultisim result object                                                                                                                                                                                                     |
| ...     | randseed: The random seed protocol: UMI or non-UMI<br>gene_len: A vector with lengths of all genes<br>alpha_mean, alpha_sd: rate of subsampling of transcripts during capture step<br>depth_mean, depth_sd: The sequencing depth |

**Value**

none

**See Also**

The underlying methods [True2ObservedCounts](#) and [True2ObservedATAC](#)

**Examples**

```
results <- sim_example(ncells = 10)
add_expr_noise(results)
```

---

|              |                                            |
|--------------|--------------------------------------------|
| add_outliers | <i>Add outliers to the observed counts</i> |
|--------------|--------------------------------------------|

---

**Description**

Add outliers to the observed counts

**Usage**

```
add_outliers(
  res,
  prob = 0.01,
  factor = 2,
  sd = 0.5,
  cell.num = 1,
  max.var = Inf
)
```

**Arguments**

|                       |                                                        |
|-----------------------|--------------------------------------------------------|
| <code>res</code>      | The scMultisim result object                           |
| <code>prob</code>     | The probability of adding outliers for each gene       |
| <code>factor</code>   | The factor of the outliers                             |
| <code>sd</code>       | The standard deviation of the outliers                 |
| <code>cell.num</code> | For a gene, the number of cells chosen to add outliers |
| <code>max.var</code>  | The maximum variance allowed                           |

**Value**

none

---

`cci_cell_type_params`    *Generate cell-type level CCI parameters*

---

**Description**

See the return value if you want to specify the cell-type level ground truth.

**Usage**

```
cci_cell_type_params(
  tree,
  total.lr,
  ctype.lr = 4:6,
  step.size = 1,
  rand = TRUE,
  discrete = FALSE
)
```

**Arguments**

|                        |                                                                                                                             |
|------------------------|-----------------------------------------------------------------------------------------------------------------------------|
| <code>tree</code>      | Use the same value for <code>sim_true_counts()</code> .                                                                     |
| <code>total.lr</code>  | Total number of LR pairs in the database. Use the same value for <code>sim_true_counts()</code> .                           |
| <code>ctype.lr</code>  | If <code>rand</code> is TRUE, how many LR pairs should be enabled between each cell type pair. Should be a range, e.g. 4:6. |
| <code>step.size</code> | Use the same value for <code>sim_true_counts()</code> .                                                                     |
| <code>rand</code>      | Whether fill the matrix randomly                                                                                            |
| <code>discrete</code>  | Whether the cell population is discrete. Use the same value for <code>sim_true_counts()</code> .                            |

**Value**

A 3D matrix of (n\_cell\_type, n\_cell\_type, n\_lr). The value at (i, j, k) is 1 if there exist CCI of LR-pair k between cell type i and cell type j.

**Examples**

```
cci_cell_type_params(Phyla3(), 100, 4:6, 0.5, TRUE, FALSE)
```

---

|              |                                                                                                                              |
|--------------|------------------------------------------------------------------------------------------------------------------------------|
| dens_nonzero | <i>this is the density function of <math>\log(x+1)</math>, where <math>x</math> is the non-zero values for ATAC-SEQ data</i> |
|--------------|------------------------------------------------------------------------------------------------------------------------------|

---

**Description**

this is the density function of  $\log(x+1)$ , where  $x$  is the non-zero values for ATAC-SEQ data

**Usage**

```
data(dens_nonzero)
```

**Format**

a vector.

**Value**

a vector.

**Examples**

```
data(dens_nonzero)
```

---

|                |                                           |
|----------------|-------------------------------------------|
| divide_batches | <i>Divide batches for observed counts</i> |
|----------------|-------------------------------------------|

---

**Description**

Divide batches for observed counts

**Usage**

```
divide_batches(results, nbatch = 2, effect = 3, randseed = 0)
```

**Arguments**

|          |                                                            |
|----------|------------------------------------------------------------|
| results  | The scMultisim result object, after running addExprNoise() |
| nbatch   | Number of batches                                          |
| effect   | Batch effect size, default is 3                            |
| randseed | Random seed                                                |

**Value**

none

**Examples**

```
results <- sim_example(ncells = 10)
add_expr_noise(results)
divide_batches(results)
```

---

gene\_corr\_cci

*Plot the ligand-receptor correlation summary*

---

**Description**

Plot the ligand-receptor correlation summary

**Usage**

```
gene_corr_cci(
  results = .getResultsFromGlobal(),
  all.genes = FALSE,
  .pair = NULL,
  .exclude.same.types = TRUE
)
```

**Arguments**

|                     |                                                            |
|---------------------|------------------------------------------------------------|
| results             | The scMultisim result object                               |
| all.genes           | Whether to use all genes or only the ligand/receptor genes |
| .pair               | Return the raw data for the given LR pair                  |
| .exclude.same.types | Whether to exclude neighbor cells with same cell type      |

**Value**

none

**Examples**

```
results <- sim_example_spatial(ncells = 10)
gene_corr_cci(results)
```

---

|                     |                                                                 |
|---------------------|-----------------------------------------------------------------|
| gene_corr_regulator | <i>Print the correlations between targets of each regulator</i> |
|---------------------|-----------------------------------------------------------------|

---

**Description**

Print the correlations between targets of each regulator

**Usage**

```
gene_corr_regulator(results = .getResultsFromGlobal(), regulator)
```

**Arguments**

|           |                                    |
|-----------|------------------------------------|
| results   | The scMultisim result object       |
| regulator | The regulator ID in the GRN params |

**Value**

none

**Examples**

```
results <- sim_example(ncells = 10)
gene_corr_regulator(results, 2)
```

---

|               |                                              |
|---------------|----------------------------------------------|
| gene_len_pool | <i>a pool of gene lengths to sample from</i> |
|---------------|----------------------------------------------|

---

**Description**

a pool of gene lengths to sample from

**Usage**

```
data(gene_len_pool)
```

**Format**

a vector.

**Value**

a vector of gene lengths.

**Examples**

```
data(gene_len_pool)
```

---

gen\_1branch

---

*Generate true transcript counts for linear structure*


---

### Description

Generate true transcript counts for linear structure

### Usage

```
gen_1branch(
  kinet_params,
  start_state,
  start_s,
  start_u,
  randpoints1,
  ncells1,
  ngenes,
  beta_vec,
  d_vec,
  cycle_length_factor,
  cell
)
```

### Arguments

|                     |                                                                                                                                                              |
|---------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------|
| kinet_params        | kinetic parameters, include k_on, k_off, s and beta                                                                                                          |
| start_state         | the starting state: on or off of each gene                                                                                                                   |
| start_s             | spliced count of the root cell in the branch                                                                                                                 |
| start_u             | unspliced count of the root cell in the branch                                                                                                               |
| randpoints1         | the value which evf mean is generated from                                                                                                                   |
| ncells1             | number of cells in the branch                                                                                                                                |
| ngenes              | number of genes                                                                                                                                              |
| beta_vec            | splicing rate of each gene                                                                                                                                   |
| d_vec               | degradation rate of each gene                                                                                                                                |
| cycle_length_factor | for generating velocity data, a factor which is multiplied by the expected time to transition from kon to koff and back to to form the the length of a cycle |
| cell                | the cell number currently having counts generated                                                                                                            |

### Value

a list of 4 elements, the first element is true counts, second is the gene level meta information, the third is cell level meta information, including a matrix of evf and a vector of cell identity, and the fourth is the parameters kon, koff and s used to simulation the true counts

---

|             |                                                               |
|-------------|---------------------------------------------------------------|
| gen_clutter | <i>generate a clutter of cells by growing from the center</i> |
|-------------|---------------------------------------------------------------|

---

### Description

generate a clutter of cells by growing from the center

### Usage

```
gen_clutter(
  n_cell,
  grid_size = NA,
  center = c(0, 0),
  existing_loc = NULL,
  existing_grid = NULL
)
```

### Arguments

|               |                                                      |
|---------------|------------------------------------------------------|
| n_cell        | the number of cells                                  |
| grid_size     | the width and height of the grid                     |
| center        | the center of the grid                               |
| existing_loc  | only place cells on the specified existing locations |
| existing_grid | manually specify what locations are in the grid      |

### Value

a matrix of locations

### Examples

```
gen_clutter(10, 10, c(5, 5))
```

---

Get\_1region\_ATAC\_correlation

*This function gets the average correlation rna seq counts and region effect on genes for genes which are only associated with 1 chromatin region*

---

### Description

This function gets the average correlation rna seq counts and region effect on genes for genes which are only associated with 1 chromatin region

**Usage**

```
Get_1region_ATAC_correlation(counts, atacseq_data, region2gene)
```

**Arguments**

|              |                                                                                                                                                             |
|--------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------|
| counts       | rna seq counts                                                                                                                                              |
| atacseq_data | atac seq data                                                                                                                                               |
| region2gene  | a 0 1 coupling matrix between regions and genes of shape (nregions) x (num_genes), where a value of 1 indicates the gene is affected by a particular region |

**Value**

the correlation value

**Examples**

```
results <- sim_example(ncells = 10)
Get_1region_ATAC_correlation(results$counts, results$atacseq_data, results$region_to_gene)
```

---

Get\_ATAC\_correlation    *This function gets the average correlation rna seq counts and chromatin region effect on genes*

---

**Description**

This function gets the average correlation rna seq counts and chromatin region effect on genes

**Usage**

```
Get_ATAC_correlation(counts, atacseq_data, num_genes)
```

**Arguments**

|              |                 |
|--------------|-----------------|
| counts       | rna seq counts  |
| atacseq_data | atac seq data   |
| num_genes    | number of genes |

**Value**

the correlation value

**Examples**

```
results <- sim_example(ncells = 10)
Get_ATAC_correlation(results$counts, results$atacseq_data, results$num_genes)
```

---

|                |                                                                                                                                                                                                                                                                                              |
|----------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| GRN_params_100 | <i>100_gene_GRN is a matrix of GRN params consisting of 100 genes where: # - column 1 is the target gene ID, # - column 2 is the gene ID which acts as a transcription factor for the target (regulated) gene # - column 3 is the effect of the column 2 gene ID on the column 1 gene ID</i> |
|----------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|

---

**Description**

100\_gene\_GRN is a matrix of GRN params consisting of 100 genes where: # - column 1 is the target gene ID, # - column 2 is the gene ID which acts as a transcription factor for the target (regulated) gene # - column 3 is the effect of the column 2 gene ID on the column 1 gene ID

**Usage**

```
data(GRN_params_100)
```

**Format**

a data frame.

**Value**

a data frame with three columns: target gene ID, TF gene ID, and the effect of TF on target gene.

**Examples**

```
data(GRN_params_100)
```

---

|                 |                                                                                                                                                                                                                                                                                                  |
|-----------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| GRN_params_1139 | <i>GRN_params_1139 is a matrix of GRN params consisting of 1139 genes where: # - column 1 is the target gene ID, # - column 2 is the gene ID which acts as a transcription factor for the target (regulated) gene # - column 3 is the effect of the column 2 gene ID on the column 1 gene ID</i> |
|-----------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|

---

**Description**

GRN\_params\_1139 is a matrix of GRN params consisting of 1139 genes where: # - column 1 is the target gene ID, # - column 2 is the gene ID which acts as a transcription factor for the target (regulated) gene # - column 3 is the effect of the column 2 gene ID on the column 1 gene ID

**Usage**

```
data(GRN_params_1139)
```

**Format**

a data frame.

**Value**

a data frame with three columns: target gene ID, TF gene ID, and the effect of TF on target gene.

**Examples**

```
data(GRN_params_1139)
```

---

|           |                                                                                |
|-----------|--------------------------------------------------------------------------------|
| len2nfrag | <i>from transcript length to number of fragments (for the nonUMI protocol)</i> |
|-----------|--------------------------------------------------------------------------------|

---

**Description**

from transcript length to number of fragments (for the nonUMI protocol)

**Usage**

```
data(len2nfrag)
```

**Format**

a vector.

**Value**

a vector.

**Examples**

```
data(len2nfrag)
```

---

|              |                                                                                       |
|--------------|---------------------------------------------------------------------------------------|
| match_params | <i>distribution of kinetic parameters learned from the Zeisel UMI cortex datasets</i> |
|--------------|---------------------------------------------------------------------------------------|

---

**Description**

distribution of kinetic parameters learned from the Zeisel UMI cortex datasets

**Usage**

data(param\_realdata.zeisel.imputed)

**Format**

a data frame.

**Value**

a data frame.

**Examples**

data(param\_realdata.zeisel.imputed)

---

|    |                                                             |
|----|-------------------------------------------------------------|
| OP | <i>Get option from an object in the current environment</i> |
|----|-------------------------------------------------------------|

---

**Description**

Get option from an object in the current environment

**Usage**

OP(..., .name = "options")

**Arguments**

- ... the parameter name
- .name get option from this object

**Value**

the parameter value

Phyla1

*Creating a linear example tree*

---

**Description**

Creating a linear example tree

**Usage**

```
Phyla1(len = 1)
```

**Arguments**

len                      length of the tree

**Value**

a R phylo object

**Examples**

```
Phyla1(len = 1)
```

---

Phyla3

*Creating an example tree with 3 tips*

---

**Description**

Creating an example tree with 3 tips

**Usage**

```
Phyla3(plotting = FALSE)
```

**Arguments**

plotting                True for plotting the tree on console, False for no plot

**Value**

a R phylo object

**Examples**

```
Phyla3()
```

---

**Phyla5***Creating an example tree with 5 tips*

---

**Description**

Creating an example tree with 5 tips

**Usage**

```
Phyla5(plotting = FALSE)
```

**Arguments**

**plotting**            True for plotting the tree on console, False for no plot

**Value**

a R phylo object

**Examples**

```
Phyla5()
```

---

**plot\_cell\_loc***Plot cell locations*

---

**Description**

Plot cell locations

**Usage**

```
plot_cell_loc(  
  results = .getResultsFromGlobal(),  
  size = 4,  
  show.label = FALSE,  
  show.arrows = TRUE,  
  lr.pair = 1,  
  .cell.pop = NULL,  
  .locs = NULL  
)
```

**Arguments**

|             |                                                                                        |
|-------------|----------------------------------------------------------------------------------------|
| results     | The scMultisim result object                                                           |
| size        | Fig size                                                                               |
| show.label  | Show cell numbers                                                                      |
| show.arrows | Show arrows representing cell-cell interactions                                        |
| lr.pair     | The ligand-receptor pair used to plot CCI arrows results\$cci_cell_type_param[lr.pair] |
| .cell.pop   | Specify the cell population metadata                                                   |
| .locs       | Manually specify the cell locations as a 2xncells matrix                               |

**Value**

none

**Examples**

```
results <- sim_example_spatial(ncells = 10)
plot_cell_loc(results)
```

---

plot\_gene\_module\_cor\_heatmap

*Plot the gene module correlation heatmap*

---

**Description**

Plot the gene module correlation heatmap

**Usage**

```
plot_gene_module_cor_heatmap(
  results = .getResultsFromGlobal(),
  seed = 0,
  grn.genes.only = TRUE,
  save = FALSE
)
```

**Arguments**

|                |                              |
|----------------|------------------------------|
| results        | The scMultisim result object |
| seed           | The random seed              |
| grn.genes.only | Plot the GRN gens only       |
| save           | save the plot as pdf         |

**Value**

none

**Examples**

```
results <- sim_example(ncells = 10)
plot_gene_module_cor_heatmap(results)
```

---

`plot_grid`*Plot the CCI grid*

---

**Description**

In normal cases, please use `plotCellLoc` instead.

**Usage**

```
plot_grid(results = .getResultsFromGlobal())
```

**Arguments**

`results`            The `scMultisim` result object

**Value**

none

**Examples**

```
results <- sim_example_spatial(ncells = 10)
plot_grid(results)
```

---

`plot_grn`*Plot the GRN network*

---

**Description**

Plot the GRN network

**Usage**

```
plot_grn(params)
```

**Arguments**

`params`            The GRN params data frame

**Value**

none

**Examples**

```
data(GRN_params_100, envir = environment())
plot_grn(GRN_params_100)
```

---

|            |                                   |
|------------|-----------------------------------|
| plot_phyla | <i>Plot a R phylogenetic tree</i> |
|------------|-----------------------------------|

---

**Description**

Plot a R phylogenetic tree

**Usage**

```
plot_phyla(tree)
```

**Arguments**

|      |          |
|------|----------|
| tree | The tree |
|------|----------|

**Value**

none

**Examples**

```
plot_phyla(Phyla5())
```

---

|                   |                                                 |
|-------------------|-------------------------------------------------|
| plot_rna_velocity | <i>Plot RNA velocity as arrows on tSNE plot</i> |
|-------------------|-------------------------------------------------|

---

**Description**

Plot RNA velocity as arrows on tSNE plot

**Usage**

```
plot_rna_velocity(
  results = .getResultsFromGlobal(),
  velocity = results$velocity,
  perplexity = 70,
  arrow.length = 1,
  save = FALSE,
  randseed = 0,
  ...
)
```

**Arguments**

|              |                                                                                |
|--------------|--------------------------------------------------------------------------------|
| results      | The scMultiSim result object                                                   |
| velocity     | The velocity matrix, by default using the velocity matrix in the result object |
| perplexity   | The perplexity for tSNE                                                        |
| arrow.length | The length scaler of the arrow                                                 |
| save         | Whether to save the plot                                                       |
| randseed     | The random seed                                                                |
| ...          | Other parameters passed to ggplot                                              |

**Value**

The plot

**Examples**

```
results <- sim_example(ncells = 10, velocity = TRUE)
plot_rna_velocity(results, perplexity = 3)
```

---

plot\_tsne

---

*Plot t-SNE visualization of a data matrix*


---

**Description**

Plot t-SNE visualization of a data matrix

**Usage**

```
plot_tsne(
  data,
  labels,
  perplexity = 60,
  legend = "",
  plot.name = "",
  save = FALSE,
  rand.seed = 0,
  continuous = FALSE,
  labels2 = NULL,
  lim = NULL,
  runPCA = FALSE,
  alpha = 1
)
```

**Arguments**

|            |                                                                 |
|------------|-----------------------------------------------------------------|
| data       | The dxn matrix                                                  |
| labels     | A vector of length n, usually cell clusters                     |
| perplexity | Perplexity value used for t-SNE                                 |
| legend     | A list of colors for the labels                                 |
| plot.name  | The plot title                                                  |
| save       | If TRUE, save as plot.name.pdf                                  |
| rand.seed  | The random seed                                                 |
| continuous | Whether labels should be treated as continuous, e.g. pseudotime |
| labels2    | Additional label                                                |
| lim        | Specify the xlim and y lim c(x_min, x_max, y_min, y_max)        |
| runPCA     | Whether to run PCA before t-SNE                                 |
| alpha      | The alpha value for the points                                  |

**Value**

the figure if not save, otherwise save the figure as plot.name.pdf

**Examples**

```
results <- sim_example(ncells = 10)
plot_tsne(log2(results$counts + 1), results$cell_meta$pop, perplexity = 3)
```

---

run\_shiny

---

*Launch the Shiny App to configure the simulation*


---

**Description**

Launch the Shiny App to configure the simulation

**Usage**

```
run_shiny()
```

---

|           |                                              |
|-----------|----------------------------------------------|
| SampleDen | <i>sample from smoothed density function</i> |
|-----------|----------------------------------------------|

---

**Description**

sample from smoothed density function

**Usage**

```
SampleDen(nsample, den_fun, reduce.mem = FALSE)
```

**Arguments**

|            |                                                          |
|------------|----------------------------------------------------------|
| nsample    | number of samples needed                                 |
| den_fun    | density function estimated from density() from R default |
| reduce.mem | use alternative implementation to reduce memory usage    |

**Value**

a vector of samples

---

|                 |                                                                |
|-----------------|----------------------------------------------------------------|
| scmultisim_help | <i>Show detailed documentations of scMultiSim's parameters</i> |
|-----------------|----------------------------------------------------------------|

---

**Description**

Show detailed documentations of scMultiSim's parameters

**Usage**

```
scmultisim_help(topic = NULL)
```

**Arguments**

|       |                                     |
|-------|-------------------------------------|
| topic | Can be options, dynamic.GRN, or cci |
|-------|-------------------------------------|

**Value**

none

**Examples**

```
scmultisim_help()
```

---

|             |                                                                             |
|-------------|-----------------------------------------------------------------------------|
| sim_example | <i>Simulate a small example dataset with 200 cells and the 100-gene GRN</i> |
|-------------|-----------------------------------------------------------------------------|

---

**Description**

Simulate a small example dataset with 200 cells and the 100-gene GRN

**Usage**

```
sim_example(ncells = 10, velocity = FALSE)
```

**Arguments**

|          |                                                              |
|----------|--------------------------------------------------------------|
| ncells   | number of cells, please increase this number on your machine |
| velocity | whether to simulate RNA velocity                             |

**Value**

the simulation result

**Examples**

```
sim_example(ncells = 10)
```

---

|                     |                                                                                               |
|---------------------|-----------------------------------------------------------------------------------------------|
| sim_example_spatial | <i>Simulate a small example dataset with 200 cells and the 100-gene GRN, with CCI enabled</i> |
|---------------------|-----------------------------------------------------------------------------------------------|

---

**Description**

Simulate a small example dataset with 200 cells and the 100-gene GRN, with CCI enabled

**Usage**

```
sim_example_spatial(ncells = 10)
```

**Arguments**

|        |                                                              |
|--------|--------------------------------------------------------------|
| ncells | number of cells, please increase this number on your machine |
|--------|--------------------------------------------------------------|

**Value**

the simulation result

**Examples**

```
sim_example_spatial(ncells = 10)
```

---

|                 |                                                                  |
|-----------------|------------------------------------------------------------------|
| sim_true_counts | <i>Simulate true scRNA and scATAC counts from the parameters</i> |
|-----------------|------------------------------------------------------------------|

---

**Description**

Simulate true scRNA and scATAC counts from the parameters

**Usage**

```
sim_true_counts(options, return_summarized_exp = FALSE)
```

**Arguments**

options            See `scMultiSim_help()`.  
return\_summarized\_exp            Whether to return a SummarizedExperiment object.

**Value**

scMultiSim returns an environment with the following fields:

- counts: Gene-by-cell scRNA-seq counts.
- atac\_counts: Region-by-cell scATAC-seq counts.
- region\_to\_gene: Region-by-gene 0-1 matrix indicating the corresponding relationship between chromatin regions and genes.
- atacseq\_data: The "clean" scATAC-seq counts without added intrinsic noise.
- cell\_meta: A dataframe containing cell type labels and pseudotime information.
- cif: The CIF used during the simulation.
- giv: The GIV used during the simulation.
- kinetic\_params: The kinetic parameters used during the simulation.
- .grn: The GRN used during the simulation.
- .grn\$regulators: The list of TFs used by all gene-by-TF matrices.
- .grn\$geff: Gene-by-TF matrix representing the GRN used during the simulation.
- .n: Other metadata, e.g. `.n$cells` is the number of cells.

If `do.velocity` is enabled, it has these additional fields:

- unspliced\_counts: Gene-by-cell unspliced RNA counts.
- velocity: Gene-by-cell RNA velocity ground truth.
- cell\_time: The pseudotime at which the cell counts were generated.

If dynamic GRN is enabled, it has these additional fields:

- cell\_specific\_grn: A list of length `n_cells`. Each element is a gene-by-TF matrix, indicating the cell's GRN.

If cell-cell interaction is enabled, it has these additional fields:

- `grid`: The grid object used during the simulation.
  - `grid$get_neighbours(i)`: Get the neighbour cells of cell `i`.
- `cci_locs`: A dataframe containing the X and Y coordinates of each cell.
- `cci_cell_type_param`: A dataframe containing the CCI network ground truth: all ligand-receptor pairs between each pair of cell types.
- `cci_cell_types`: For continuous cell population, the sub-divided cell types along the trajectory used when simulating CCI.

If it is a debug session (`debug = TRUE`), a `sim` field is available, which is an environment contains all internal states and data structures.

### Examples

```
data(GRN_params_100, envir = environment())
sim_true_counts(list(
  rand.seed = 0,
  GRN = GRN_params_100,
  num.cells = 100,
  num.cifs = 50,
  tree = Phyla5()
))
```

---

|                   |                                    |
|-------------------|------------------------------------|
| spatialGrid-class | <i>The class for spatial grids</i> |
|-------------------|------------------------------------|

---

### Description

The class for spatial grids

### Value

a `spatialGrid` object

### Fields

`method` the method to generate the cell layout  
`grid_size` the width and height of the grid  
`ncells` the number of cells  
`grid` the grid matrix  
`locs` a list containing the locations of all cells  
`loc_order` deprecated, don't use; the order of the locations  
`cell_types` a map to save the cell type of each allocated cell  
`same_type_prob` the probability of a new cell placed next to a cell with the same type

max\_nbs the maximum number of neighbors for each cell  
 nb\_map a list containing the neighbors for each cell  
 nb\_adj adjacency matrix for neighbors  
 nb\_radius the radius of neighbors  
 final\_types the final cell types after the final time step  
 pre\_allocated\_pos the pre-allocated positions for each cell, if any  
 method\_param additional parameters for the layout method

---

|                   |                                                                                    |
|-------------------|------------------------------------------------------------------------------------|
| True2observedATAC | <i>Simulate observed ATAC-seq matrix given technical noise and the true counts</i> |
|-------------------|------------------------------------------------------------------------------------|

---

## Description

Simulate observed ATAC-seq matrix given technical noise and the true counts

## Usage

```
True2observedATAC(
  atacseq_data,
  randseed,
  observation_prob = 0.3,
  sd_frac = 0.1
)
```

## Arguments

|                  |                                                                                                                 |
|------------------|-----------------------------------------------------------------------------------------------------------------|
| atacseq_data     | true ATAC-seq data                                                                                              |
| randseed         | (should produce same result if nregions, nevf and randseed are all the same)                                    |
| observation_prob | for each integer count of a particular region for a particular cell, the probability the count will be observed |
| sd_frac          | the fraction of ATAC-seq data value used as the standard deviation of added normally distributed noise          |

## Value

a matrix of observed ATAC-seq data

## Examples

```
results <- sim_example(ncells = 10)
True2observedATAC(results$atac_counts, randseed = 1)
```

---

|                     |                                                                                  |
|---------------------|----------------------------------------------------------------------------------|
| True2ObservedCounts | <i>Simulate observed count matrix given technical biases and the true counts</i> |
|---------------------|----------------------------------------------------------------------------------|

---

## Description

Simulate observed count matrix given technical biases and the true counts

## Usage

```
True2ObservedCounts(
  true_counts,
  meta_cell,
  protocol,
  randseed,
  alpha_mean = 0.1,
  alpha_sd = 0.002,
  alpha_gene_mean = 1,
  alpha_gene_sd = 0,
  gene_len,
  depth_mean,
  depth_sd,
  lenslope = 0.02,
  nbins = 20,
  amp_bias_limit = c(-0.2, 0.2),
  rate_2PCR = 0.8,
  nPCR1 = 16,
  nPCR2 = 10,
  LinearAmp = FALSE,
  LinearAmp_coef = 2000
)
```

## Arguments

|                 |                                                                                                            |
|-----------------|------------------------------------------------------------------------------------------------------------|
| true_counts     | gene cell matrix                                                                                           |
| meta_cell       | the meta information related to cells, will be combined with technical cell level information and returned |
| protocol        | a string, can be "nonUMI" or "UMI"                                                                         |
| randseed        | (should produce same result if nregions, nev and randseed are all the same)                                |
| alpha_mean      | the mean of rate of subsampling of transcripts during capture step, default at 10 percent efficiency       |
| alpha_sd        | the std of rate of subsampling of transcripts                                                              |
| alpha_gene_mean | the per-gene scale factor of the alpha parameter, default at 1                                             |

|                             |                                                                                                |
|-----------------------------|------------------------------------------------------------------------------------------------|
| <code>alpha_gene_sd</code>  | the standard deviation of the per-gene scale factor of the alpha parameter, default at 0       |
| <code>gene_len</code>       | a vector with lengths of all genes                                                             |
| <code>depth_mean</code>     | mean of sequencing depth                                                                       |
| <code>depth_sd</code>       | std of sequencing depth                                                                        |
| <code>lenslope</code>       | amount of length bias                                                                          |
| <code>nbins</code>          | number of bins for gene length                                                                 |
| <code>amp_bias_limit</code> | range of amplification bias for each gene, a vector of length ngenes                           |
| <code>rate_2PCR</code>      | PCR efficiency, usually very high, default is 0.8                                              |
| <code>nPCR1</code>          | the number of PCR cycles in "pre-amplification" step, default is 16                            |
| <code>nPCR2</code>          | the number of PCR cycles used after fragmentation.                                             |
| <code>LinearAmp</code>      | if linear amplification is used for pre-amplification step, default is FALSE                   |
| <code>LinearAmp_coef</code> | the coefficient of linear amplification, that is, how many times each molecule is amplified by |

**Value**

if UMI, a list with two elements, the first is the observed count matrix, the second is the metadata;  
if nonUMI, a matrix

**Examples**

```
results <- sim_example(ncells = 10)
data(gene_len_pool)
gene_len <- sample(gene_len_pool, results$num_genes, replace = FALSE)
True2ObservedCounts(
  results$counts, results$cell_meta, protocol = "nonUMI", randseed = 1,
  alpha_mean = 0.1, alpha_sd = 0.05, gene_len = gene_len, depth_mean = 1e5, depth_sd = 3e3
)
```

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