

# Package ‘simPIC’

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**Type** Package

**Title** Flexible simulation of paired-insertion counts for single-cell ATAC-sequencing data

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**Description** simPIC is a package for simulating single-cell ATAC-seq count data. It provides a user-friendly, well documented interface for data simulation. Functions are provided for parameter estimation, realistic scATAC-seq data simulation, and comparing real and simulated datasets.

**biocViews** SingleCell, ATACSeq, Software, Sequencing, ImmunoOncology, DataImport

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**Config/testthat/edition** 3

**URL** <https://github.com/sagrikachugh/simPIC>

**BugReports** <https://github.com/sagrikachugh/simPIC/issues>

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|                |                                                                                                    |
|----------------|----------------------------------------------------------------------------------------------------|
| simPIC-package | <i>simPIC: Flexible simulation of paired-insertion counts for single-cell ATAC-sequencing data</i> |
|----------------|----------------------------------------------------------------------------------------------------|

---

## Description

simPIC is a package for simulating single-cell ATAC-seq count data. It provides a user-friendly, well documented interface for data simulation. Functions are provided for parameter estimation, realistic scATAC-seq data simulation, and comparing real and simulated datasets.

- count class ([newsimPICcount](#))
- estimate ([simPICEstimate](#))
- simulate ([simPICsimulate](#))
- plots ([simPICcompare](#))

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- Davis McCarthy

**See Also**

Useful links:

- <https://github.com/sagrikachugh/simPIC>
- Report bugs at <https://github.com/sagrikachugh/simPIC/issues>

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|                 |                               |
|-----------------|-------------------------------|
| addFeatureStats | <i>Add feature statistics</i> |
|-----------------|-------------------------------|

---

**Description**

Add additional feature statistics to a SingleCellExperiment object

**Usage**

```
addFeatureStats(  
  sce,  
  value = "counts",  
  log = FALSE,  
  offset = 1,  
  no.zeros = FALSE  
)
```

**Arguments**

|          |                                                                                       |
|----------|---------------------------------------------------------------------------------------|
| sce      | SingleCellExperiment to add feature statistics to.                                    |
| value    | the count value to calculate statistics.                                              |
| log      | logical. Whether to take log2 before calculating statistics.                          |
| offset   | offset to add to avoid taking log of zero.                                            |
| no.zeros | logical. Whether to remove all zeros from each feature before calculating statistics. |

**Details**

Currently adds the following statistics: mean and variance. Statistics are added to the `rowData` slot and are named `Stat[Log]Value[No0]` where Log and No0 are added if those arguments are true.

**Value**

SingleCellExperiment with additional feature statistics

---

|                |                                                             |
|----------------|-------------------------------------------------------------|
| convert_to_SCE | <i>Convert Sparse Matrix to SingleCellExperiment object</i> |
|----------------|-------------------------------------------------------------|

---

### Description

This function converts a sparse matrix into a SingleCellExperiment(SCE) object.

### Usage

```
convert_to_SCE(sparse_data)
```

### Arguments

|             |                                                                                          |
|-------------|------------------------------------------------------------------------------------------|
| sparse_data | A sparse matrix containing count data, where rows are peaks and columns represent cells. |
|-------------|------------------------------------------------------------------------------------------|

### Value

A SingleCellExperiment(SCE) object with the sparse matrix stored in the "counts" assay.

---

|           |                                                      |
|-----------|------------------------------------------------------|
| getCounts | <i>Get counts from Single Cell Experiment object</i> |
|-----------|------------------------------------------------------|

---

### Description

Get counts matrix from a SingleCellExperiment object. If counts is missing a warning is issued and the first assay is returned.

### Usage

```
getCounts(sce)
```

### Arguments

|     |                             |
|-----|-----------------------------|
| sce | SingleCellExperiment object |
|-----|-----------------------------|

### Value

counts matrix

---

|                 |                                  |
|-----------------|----------------------------------|
| getLNormFactors | <i>Get accessibility factors</i> |
|-----------------|----------------------------------|

---

**Description**

Randomly generate multiplication factors from a log-normal distribution.

**Usage**

```
getLNormFactors(n.facs, sel.prob, neg.prob, fac.loc, fac.scale)
```

**Arguments**

|           |                                                                    |
|-----------|--------------------------------------------------------------------|
| n.facs    | Number of factors to generate.                                     |
| sel.prob  | Probability that a factor will be selected to be different from 1. |
| neg.prob  | Probability that a selected factor is less than one.               |
| fac.loc   | Location parameter for the log-normal distribution.                |
| fac.scale | Scale factor for the log-normal distribution.                      |

**Value**

Vector containing generated factors.

---

|        |                                                   |
|--------|---------------------------------------------------|
| global | <i>simPIC: Simulate single-cell ATAC-seq data</i> |
|--------|---------------------------------------------------|

---

**Description**

simPIC: Simulate single-cell ATAC-seq data

**Value**

globalvariables

---

|                |                       |
|----------------|-----------------------|
| newsimPICcount | <i>newsimPICcount</i> |
|----------------|-----------------------|

---

**Description**

Create a newsimPICcount object to store parameters.

**Usage**

```
newsimPICcount(...)
```

**Arguments**

... Variables to set newsimPICcount object parameters.

**Details**

This function creates the object variable which is passed in all functions.

**Value**

new object from class simPICcount.

**Examples**

```
object <- newsimPICcount()
```

---

|            |                                 |
|------------|---------------------------------|
| plot_theme | <i>Custom theme for ggplot2</i> |
|------------|---------------------------------|

---

**Description**

This function defines a custom theme for ggplot2 to ensure consistent visual appearance across multiple plots.

**Usage**

```
plot_theme()
```

**Value**

A ggplot2 theme object with predefined settings.

---

|              |                            |
|--------------|----------------------------|
| rbindMatched | <i>Bind rows (matched)</i> |
|--------------|----------------------------|

---

**Description**

Bind the rows of two data frames, keeping only the columns that are common to both.

**Usage**

```
rbindMatched(df1, df2)
```

**Arguments**

|     |                            |
|-----|----------------------------|
| df1 | first data.frame to bind.  |
| df2 | second data.frame to bind. |

**Value**

data.frame containing rows from df1 and df2 but only common columns.

---

|           |                   |
|-----------|-------------------|
| selectFit | <i>Select fit</i> |
|-----------|-------------------|

---

**Description**

Trying two fitting methods and selecting the best one.

**Usage**

```
selectFit(data, distr, verbose = TRUE)
```

**Arguments**

|         |                                    |
|---------|------------------------------------|
| data    | The data to fit.                   |
| distr   | Name of the distribution to fit.   |
| verbose | logical. To print messages or not. |

**Details**

The distribution is fitted to the data using each of the [fitdist](#) fitting methods. The fit with the smallest Cramer-von Mises statistic is selected.

**Value**

The selected fit object

---

|                     |                              |
|---------------------|------------------------------|
| setsimPICparameters | <i>Set simPIC parameters</i> |
|---------------------|------------------------------|

---

### Description

Set input parameters of the simPICcount object.

### Usage

```
setsimPICparameters(object, update = NULL, ...)
```

### Arguments

|        |                                            |
|--------|--------------------------------------------|
| object | input simPICcount object.                  |
| update | new parameters.                            |
| ...    | set new parameters for simPICcount object. |

### Value

simPICcount object with updated parameters.

### Examples

```
object <- newsimPICcount()
object <- setsimPICparameters(object, nCells = 200, nPeaks = 500)
```

---

|               |                                             |
|---------------|---------------------------------------------|
| simPICcompare | <i>Compare SingleCellExperiment objects</i> |
|---------------|---------------------------------------------|

---

### Description

Combine data from several SingleCellExperiment objects and produce some basic plots comparing them.

### Usage

```
simPICcompare(
  sces,
  point.size = 0.2,
  point.alpha = 0.1,
  fits = TRUE,
  colours = NULL
)
```



## Arguments

|                          |                                                                    |
|--------------------------|--------------------------------------------------------------------|
| <code>scs</code>         | named list of SingleCellExperiment objects to combine and compare. |
| <code>point.size</code>  | size of points in scatter plots.                                   |
| <code>point.alpha</code> | opacity of points in scatter plots.                                |
| <code>fits</code>        | whether to include fits in scatter plots.                          |
| <code>colours</code>     | vector of colours to use for each dataset.                         |

## Details

The returned list has three items:

`RowData` Combined row data from the provided SingleCellExperiments.

`ColData` Combined column data from the provided SingleCellExperiments.

`Plots` Comparison plots

`Means` Boxplot of mean distribution.

`Variances` Boxplot of variance distribution.

`MeanVar` Scatter plot with fitted lines showing the mean-variance relationship.

`LibrarySizes` Boxplot of the library size distribution.

`ZerosPeak` Boxplot of the percentage of each peak that is zero.

`ZerosCell` Boxplot of the percentage of each cell that is zero.

`MeanZeros` Scatter plot with fitted lines showing the mean-zeros relationship.

The plots returned by this function are created using [ggplot](#) and are only a sample of the kind of plots you might like to consider. The data used to create these plots is also returned and should be in the correct format to allow you to create further plots using [ggplot](#).

## Value

List containing the combined datasets and plots.

## Examples

```
sim1 <- simPICsimulate(
  nPeaks = 1000, nCells = 500,
  pm.distr = "weibull", seed = 7856
)
sim2 <- simPICsimulate(
  nPeaks = 1000, nCells = 500,
  pm.distr = "gamma", seed = 4234
)
comparison <- simPICcompare(list(weibull = sim1, gamma = sim2))
names(comparison)
names(comparison$Plots)
```

---

|             |                              |
|-------------|------------------------------|
| simPICcount | <i>The simPICcount class</i> |
|-------------|------------------------------|

---

### Description

S4 class that holds parameters for simPIC simulation.

### Value

a simPIC class object. The parameters not shown in brackets can be estimated from real data using [simPICEstimate](#). For details of the simPIC simulation see [simPICsimulate](#). The default parameters are based on PBMC10k dataset and can be reproduced using test data and script provided in inst/script

### Parameters

simPIC simulation parameters:

nPeaks The number of peaks to simulate.

nCells The number of cells to simulate.

[seed] Seed to use for generating random numbers.

[default] The logical variable whether to use default parameters (TRUE) or learn from data (FALSE)

**Library size parameters** lib.size.meanlog meanlog (location) parameter for the library size log-normal distribution.

lib.size.sdlog sdlog (scale) parameter for the library size log-normal distribution.

**Peak mean parameters** mean.scale scale parameter for the mean weibull distribution.

mean.shape shape parameter for the mean weibull distribution.

**Cell sparsity parameters** sparsity probability of openness to be multiplied to the input of poisson distribution to generate final simulated matrix.

---

|              |                                                                       |
|--------------|-----------------------------------------------------------------------|
| simPICEstBCV | <i>Estimate simPIC Biological Coefficient of Variation parameters</i> |
|--------------|-----------------------------------------------------------------------|

---

### Description

Parameters are estimated using the [estimateDisp](#) function in the edgeR package.

### Usage

```
simPICEstBCV(counts, object, verbose)
```

### Arguments

counts counts matrix to estimate parameters from.

object simPICcount object to store estimated values in.

verbose logical. To print progress messages or not.

## Details

The `estimateDisp` function is used to estimate the common dispersion and prior degrees of freedom. See `estimateDisp` for details. When estimating parameters on simulated data we found a broadly linear relationship between the true underlying common dispersion and the edgeR estimate, therefore we apply a small correction,  $\text{disp} = -0.3 + 0.15 \times \text{edgeR.disp}$ .

## Value

simPICcount object with estimated values.

---

|                |                                              |
|----------------|----------------------------------------------|
| simPICestimate | <i>Estimate simPIC simulation parameters</i> |
|----------------|----------------------------------------------|

---

## Description

Estimate simulation parameters for library size, peak means, and sparsity for simPIC simulation from a real peak by cell input matrix

## Usage

```
simPICestimate(
  counts,
  object = newsimPICcount(),
  pm.distr = c("gamma", "weibull", "pareto", "lgamma"),
  method = c("single", "groups"),
  verbose = TRUE
)

## S3 method for class 'SingleCellExperiment'
simPICestimate(
  counts,
  object = newsimPICcount(),
  pm.distr = "weibull",
  method = "single",
  verbose = TRUE
)

## S3 method for class 'dgCMatix'
simPICestimate(
  counts,
  object = newsimPICcount(),
  pm.distr = "weibull",
  method = "single",
  verbose = TRUE
)
```

## Arguments

|        |                                                                                                                           |
|--------|---------------------------------------------------------------------------------------------------------------------------|
| counts | either a sparse peak by cell count matrix, or a SingleCellExperiment object containing count data to estimate parameters. |
| object | simPICcount object to store estimated parameters and counts.                                                              |

|          |                                                                                                                                             |
|----------|---------------------------------------------------------------------------------------------------------------------------------------------|
| pm.distr | statistical distribution for estimating peak mean parameters. Available distributions: gamma, weibull, lngamma, pareto. Default is weibull. |
| method   | to use for simulation. Single for simulating one cell-type or groups for simulating distinct cell-types.                                    |
| verbose  | logical variable. Prints the simulation progress if TRUE.                                                                                   |

**Value**

simPICcount object containing all estimated parameters.

**Examples**

```
counts <- readRDS(system.file("extdata", "test.rds", package = "simPIC"))
est <- newsimPICcount()
est <- simPICestimate(counts, pm.distr = "weibull")
```

---

simPICestimateLibSize *Estimate simPIC library size parameters.*

---

**Description**

Estimate the library size parameters for simPIC simulation.

**Usage**

```
simPICestimateLibSize(counts, object, verbose)
```

**Arguments**

|         |                                               |
|---------|-----------------------------------------------|
| counts  | count matrix.                                 |
| object  | simPICcount object to store estimated values. |
| verbose | logical. To print messages or not.            |

**Details**

Parameters for the lognormal distribution are estimated by fitting the library sizes using [fitdist](#). All the fitting methods are tried and the fit with the best Cramer-von Mises statistic is selected.

**Value**

simPICcount object with estimated library size parameters.

---

`simPICestimatePeakMean`*Estimate simPIC peak means*

---

**Description**

Estimate peak mean parameters for simPIC simulation

**Usage**

```
simPICestimatePeakMean(norm.counts, object, pm.distr, verbose)
```

**Arguments**

|                          |                                               |
|--------------------------|-----------------------------------------------|
| <code>norm.counts</code> | library size normalised counts matrix.        |
| <code>object</code>      | simPICcount object to store estimated values. |
| <code>pm.distr</code>    | distribution parameter for peak means.        |
| <code>verbose</code>     | logical. To print progress messages or not.   |

**Details**

Parameters for gamma distribution are estimated by fitting the mean normalised counts using [fitdist](#). All the fitting methods are tried and the fit with the best Cramer-von Mises statistic is selected.

**Value**

simPICcount object containing all estimated parameters

---

`simPICestimateSparsity`*Estimate sparsity.*

---

**Description**

This function estimates the sparsity of cells based on a normalized counts matrix and updates the parameters of a simPIC object accordingly.

**Usage**

```
simPICestimateSparsity(norm.counts, object, verbose)
```

**Arguments**

|                          |                                                        |
|--------------------------|--------------------------------------------------------|
| <code>norm.counts</code> | A normalized count matrix to estimate parameters from. |
| <code>object</code>      | simPICcount object to store estimated parameters.      |
| <code>verbose</code>     | logical. To print messages or not.                     |

**Value**

simPICcount object with updated sparsity parameter.

---

`simPICget`*Get a single simPICcount parameter*

---

**Description**

Get the value of a single variable from input simPICcount object.

**Usage**

```
simPICget(object, name)
```

**Arguments**

|                     |                           |
|---------------------|---------------------------|
| <code>object</code> | input simPICcount object. |
| <code>name</code>   | name of the parameter.    |

**Value**

Value of the input parameter.

**Examples**

```
object <- newsimPICcount()
nPeaks <- simPICget(object, "nPeaks")
```

---

`simPICgetparameters`*Get parameters*

---

**Description**

Get multiple parameter values from a simPIC object.

**Usage**

```
simPICgetparameters(object, names)
```

**Arguments**

|                     |                                           |
|---------------------|-------------------------------------------|
| <code>object</code> | input object to get values from.          |
| <code>names</code>  | vector of names of the parameters to get. |

**Value**

List with the values of the selected parameters.

**Examples**

```
object <- newsimPICcount()
simPICgetparameters(object, c("nPeaks", "nCells", "peak.mean.shape"))
```

---

`simPICsimBatchCellMeans`*Simulate batch means*

---

**Description**

Simulate a mean for each peak in each cell incorporating batch effect factors.

**Usage**

```
simPICsimBatchCellMeans(object, sim)
```

**Arguments**

|                     |                                                |
|---------------------|------------------------------------------------|
| <code>object</code> | simPICcount object with simulation parameters. |
| <code>sim</code>    | SingleCellExperiment to add batch means to.    |

**Value**

SingleCellExperiment with simulated batch means.

---

`simPICsimBatchEffects` *Simulate batch effects*

---

**Description**

Simulate batch effects. Batch effect factors for each batch are produced using [getLNormFactors](#) and these are added along with updated means for each batch.

**Usage**

```
simPICsimBatchEffects(object, sim)
```

**Arguments**

|                     |                                                |
|---------------------|------------------------------------------------|
| <code>object</code> | simPICcount object with simulation parameters. |
| <code>sim</code>    | SingleCellExperiment to add batch effects to.  |

**Value**

SingleCellExperiment with simulated batch effects.

---

|                    |                            |
|--------------------|----------------------------|
| simPICsimCellMeans | <i>Simulate cell means</i> |
|--------------------|----------------------------|

---

### Description

Simulate a peak by cell matrix given the mean accessibility for each peak in each cell. Cells start with the mean accessibility for the group they belong to (when simulating groups). The selected means are adjusted for each cell's expected library size.

### Usage

```
simPICsimSingleCellMeans(object, sim)

simPICsimulateGroupCellMeans(object, sim)
```

### Arguments

|        |                                            |
|--------|--------------------------------------------|
| object | simPIC object with simulation parameters.  |
| sim    | SingleCellExperiment to add cell means to. |

### Value

SingleCellExperiment with added cell means.

---

|                |                          |
|----------------|--------------------------|
| simPICsimulate | <i>simPIC simulation</i> |
|----------------|--------------------------|

---

### Description

Simulate peak by cell count matrix from a sparse single-cell ATAC-seq peak by cell input using simPIC methods.

### Usage

```
simPICsimulate(
  object = newsimPICcount(),
  pm.distr = "weibull",
  method = c("single", "groups"),
  verbose = TRUE,
  ...
)

simPICsimulatesingle(object = newsimPICcount(), verbose = TRUE, ...)

simPICsimulatemulti(
  object = newsimPICcount(),
  pm.distr = "weibull",
  method = c("groups"),
  verbose = TRUE,
  ...
)
```



**Arguments**

|          |                                                                                                                      |
|----------|----------------------------------------------------------------------------------------------------------------------|
| object   | simPICcount object with simulation parameters. See <a href="#">simPICcount</a> for details.                          |
| pm.distr | distribution parameter for peak means. Available distributions: gamma, weibull, lngamma, pareto. Default is weibull. |
| method   | to use for simulation. Single for simulating one cell-type or groups for simulating distinct cell-types.             |
| verbose  | logical variable. Prints the simulation progress if TRUE.                                                            |
| ...      | Any additional parameter settings to override what is provided in simPICcount object.                                |

**Details**

simPIC provides the option to manually adjust each of the simPICcount object parameters by calling [setsimPICparameters](#).

The simulation involves following steps:

1. Set up simulation parameters
2. Set up SingleCellExperiment object
3. Simulate library sizes
4. Simulate sparsity
5. Simulate peak means
6. Create final synthetic counts

The final output is a [SingleCellExperiment](#) object that contains the simulated count matrix. The parameters are stored in the [colData](#) (for cell specific information), [rowData](#) (for peak specific information) or [assays](#) (for peak by cell matrix) slots. This additional information includes:

**Value**

SingleCellExperiment object containing the simulated counts.

**Examples**

```
# default simulation
sim <- simPICsimulate(pm.distr = "weibull")
```

---

simPICsimulateBCVMeans

*Simulate BCV means*

---

**Description**

Simulate means for each peak in each cell that are adjusted to follow a mean-variance trend using Biological Coefficient of Variation taken from and inverse gamma distribution.

**Usage**

```
simPICsimulateBCVMeans(object, sim)
```

**Arguments**

|        |                                                |
|--------|------------------------------------------------|
| object | simPICcount object with simulation parameters. |
| sim    | SingleCellExperiment to add BCV means to.      |

**Value**

SingleCellExperiment with simulated BCV means.

---

simPICsimulateLibSize *Simulate simPIC library sizes*

---

**Description**

Generate library sizes for cells in simPIC simulation based on the estimated values of mus and sigmas.

**Usage**

```
simPICsimulateLibSize(object, sim, verbose)
```

**Arguments**

|         |                                                               |
|---------|---------------------------------------------------------------|
| object  | simPICcount object with simulation parameters.                |
| sim     | SingleCellExperiment object containing simulation parameters. |
| verbose | logical. To print progress messages.                          |

**Value**

SingleCellExperiment object with simulated library sizes.

---

simPICsimulatemultiDA *Simulate group differential accessibility*

---

**Description**

Simulate differential accessibility. Differential accessibility factors for each group are produced using [getLNormFactors](#) and these are added along with updated means for each group. For paths care is taken to make sure they are simulated in the correct order.

**Usage**

```
simPICsimulatemultiDA(object, sim)
```

**Arguments**

|        |                                                            |
|--------|------------------------------------------------------------|
| object | simPICcount object with simulation parameters.             |
| sim    | SingleCellExperiment to add differential accessibility to. |

**Value**

SingleCellExperiment with simulated differential accessibility.

---

```
simPICsimulatePeakMean
```

*Simulate simPIC peak means.*

---

### Description

Generate peak means for cells in simPIC simulation based on the estimated values of shape and rate parameters.

### Usage

```
simPICsimulatePeakMean(object, sim, pm.distr, verbose)
```

### Arguments

|          |                                                                                                                      |
|----------|----------------------------------------------------------------------------------------------------------------------|
| object   | simPICcount object with simulation parameters.                                                                       |
| sim      | SingleCellExperiment object containing simulation parameters.                                                        |
| pm.distr | distribution parameter for peak means. Available distributions: gamma, weibull, lngamma, pareto. Default is weibull. |
| verbose  | logical. Whether to print progress messages.                                                                         |

### Value

SingleCellExperiment object with simulated peak means.

---

```
simPICsimulateTrueCounts
```

*Simulate true counts.*

---

### Description

Counts are simulated from a poisson distribution where each peak has a mean, expected library size and proportion of accessible chromatin.

### Usage

```
simPICsimulateTrueCounts(object, sim)
```

### Arguments

|        |                                                               |
|--------|---------------------------------------------------------------|
| object | simPICcount object with simulation parameters.                |
| sim    | SingleCellExperiment object containing simulation parameters. |

### Value

SingleCellExperiment object with simulated true counts.

---

`simPICsimulateTrueCountsGroups`*Simulate true counts groups.*

---

**Description**

Counts are simulated from a poisson distribution where each peak has a mean, expected library size and proportion of accessible chromatin.

**Usage**

```
simPICsimulateTrueCountsGroups(object, sim)
```

**Arguments**

|                     |                                                               |
|---------------------|---------------------------------------------------------------|
| <code>object</code> | simPICcount object with simulation parameters.                |
| <code>sim</code>    | SingleCellExperiment object containing simulation parameters. |

**Value**

SingleCellExperiment object with simulated true counts.

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