

Package ‘SIMLR’

January 21, 2025

Version 1.32.0

Date 2024-09-20

Title Single-cell Interpretation via Multi-kernel LeaRning (SIMLR)

Depends R (>= 4.1.0),

Imports parallel, Matrix, stats, methods, Rcpp, pracma, RcppAnnoy,
RSpectra

Suggests BiocGenerics, BiocStyle, testthat, knitr, igraph

Description Single-cell RNA-seq technologies enable high throughput gene expression measurement of individual cells, and allow the discovery of heterogeneity within cell populations. Measurement of cell-to-cell gene expression similarity is critical for the identification, visualization and analysis of cell populations. However, single-cell data introduce challenges to conventional measures of gene expression similarity because of the high level of noise, outliers and dropouts. We develop a novel similarity-learning framework, SIMLR (Single-cell Interpretation via Multi-kernel LeaRning), which learns an appropriate distance metric from the data for dimension reduction, clustering and visualization.

Encoding UTF-8

License file LICENSE

URL <https://github.com/BatzoglouLabSU/SIMLR>

BugReports <https://github.com/BatzoglouLabSU/SIMLR>

biocViews ImmunoOncology, Clustering, GeneExpression, Sequencing,
SingleCell

RoxygenNote 7.3.2

LinkingTo Rcpp

NeedsCompilation yes

VignetteBuilder knitr

git_url <https://git.bioconductor.org/packages/SIMLR>

git_branch RELEASE_3_20

git_last_commit 866063e

git_last_commit_date 2024-10-29

Repository Bioconductor 3.20

Date/Publication 2025-01-20

Author Daniele Ramazzotti [aut] (<<https://orcid.org/0000-0002-6087-2666>>),
 Bo Wang [aut],
 Luca De Sano [cre, aut] (<<https://orcid.org/0000-0002-9618-3774>>),
 Serafim Batzoglou [ctb]

Maintainer Luca De Sano <luca.desano@gmail.com>

Contents

BuettnerFlorian	2
SIMLR	3
SIMLR_Estimate_Number_of_Clusters	4
SIMLR_Feature_Ranking	4
SIMLR_Large_Scale	5
ZeiselAmit	6
Index	7

BuettnerFlorian	<i>test dataset for SIMLR</i>
-----------------	-------------------------------

Description

example dataset to test SIMLR from the work by Buettner, Florian, et al.

Usage

```
data(BuettnerFlorian)
```

Format

gene expression measurements of individual cells

Value

list of 6: `in_X` = input dataset as an (m x n) gene expression measurements of individual cells, `n_clust` = number of clusters (number of distinct true labels), `true_labs` = ground true of cluster assignments for each of the `n_clust` clusters, `seed` = seed used to compute the results for the example, `results` = result by SIMLR for the inputs defined as described, `nmi` = normalized mutual information as a measure of the inferred clusters compared to the true labels

Source

Buettner, Florian, et al. "Computational analysis of cell-to-cell heterogeneity in single-cell RNA-sequencing data reveals hidden subpopulations of cells." *Nature biotechnology* 33.2 (2015): 155-160.

SIMLR

*SIMLR***Description**

perform the SIMLR clustering algorithm

Usage

```
SIMLR(
  X,
  c,
  no.dim = NA,
  k = 10,
  if.impute = FALSE,
  normalize = FALSE,
  cores.ratio = 1
)
```

Arguments

<code>X</code>	an (m x n) data matrix of gene expression measurements of individual cells or and object of class <code>SCESet</code>
<code>c</code>	number of clusters to be estimated over <code>X</code>
<code>no.dim</code>	number of dimensions
<code>k</code>	tuning parameter
<code>if.impute</code>	should I transpose the input data?
<code>normalize</code>	should I normalize the input data?
<code>cores.ratio</code>	ratio of the number of cores to be used when computing the multi-kernel

Value

clusters the cells based on SIMLR and their similarities

list of 8 elements describing the clusters obtained by SIMLR, of which `y` are the resulting clusters: `y` = results of k-means clusterings, `S` = similarities computed by SIMLR, `F` = results from network diffusion, `ydata` = data referring the the results by k-means, `alphaK` = clustering coefficients, `execution.time` = execution time of the present run, `converge` = iterative convergence values by T-SNE, `LF` = parameters of the clustering

Examples

```
data(BuettnerFlorian)
SIMLR(X = BuettnerFlorian$in_X, c = BuettnerFlorian$n_clust, cores.ratio = 0)
```

SIMLR_Estimate_Number_of_Clusters

SIMLR Estimate Number of Clusters

Description

estimate the number of clusters by means of two heuristics as discussed in the SIMLR paper

Usage

```
SIMLR_Estimate_Number_of_Clusters(X, NUMC = 2:5, cores.ratio = 1)
```

Arguments

X	an (m x n) data matrix of gene expression measurements of individual cells
NUMC	vector of number of clusters to be considered
cores.ratio	ratio of the number of cores to be used when computing the multi-kernel

Value

a list of 2 elements: K1 and K2 with an estimation of the best clusters (the lower values the better) as discussed in the original paper of SIMLR

Examples

```
data(BuettnerFlorian)
SIMLR_Estimate_Number_of_Clusters(BuettnerFlorian$in_X,
  NUMC = 2:5,
  cores.ratio = 0)
```

SIMLR_Feature_Ranking *SIMLR Feature Ranking*

Description

perform the SIMLR feature ranking algorithm. This takes as input the original input data and the corresponding similarity matrix computed by SIMLR

Usage

```
SIMLR_Feature_Ranking(A, X)
```

Arguments

A	an (n x n) similarity matrix by SIMLR
X	an (m x n) data matrix of gene expression measurements of individual cells

Value

a list of 2 elements: pvalues and ranking ordering over the n covariates as estimated by the method

Examples

```
data(BuettnerFlorian)
SIMLR_Feature_Ranking(A = BuettnerFlorian$results$S, X = BuettnerFlorian$in_X)
```

SIMLR_Large_Scale *SIMLR Large Scale*

Description

perform the SIMLR clustering algorithm for large scale datasets

Usage

```
SIMLR_Large_Scale(X, c, k = 10, kk = 100, if.impute = FALSE, normalize = FALSE)
```

Arguments

X	an (m x n) data matrix of gene expression measurements of individual cells or and object of class SCESet
c	number of clusters to be estimated over X
k	tuning parameter
kk	number of principal components to be assessed in the PCA
if.impute	should I transpose the input data?
normalize	should I normalize the input data?

Value

clusters the cells based on SIMLR Large Scale and their similarities

list of 8 elements describing the clusters obtained by SIMLR, of which y are the resulting clusters: y = results of k-means clusterings, S0 = similarities computed by SIMLR, F = results from the large scale iterative procedure, ydata = data referring the the results by k-means, alphaK = clustering coefficients, val = distances from the k-nearest neighbour search, ind = indeces from the k-nearest neighbour search, execution.time = execution time of the present run

Examples

```
data(ZeiselAmit)
resized = ZeiselAmit$in_X[, 1:340]

SIMLR_Large_Scale(X = resized, c = ZeiselAmit$n_clust, k = 5, kk = 5)
```

ZeiselAmit

test dataset for SIMLR large scale

Description

example dataset to test SIMLR large scale. This is a reduced version of the dataset from the work by Zeisel, Amit, et al.

Usage

```
data(ZeiselAmit)
```

Format

gene expression measurements of individual cells

Value

list of 6: `in_X` = input dataset as an (m x n) gene expression measurements of individual cells, `n_clust` = number of clusters (number of distinct true labels), `true_labs` = ground true of cluster assignments for each of the `n_clust` clusters, `seed` = seed used to compute the results for the example, `results` = result by SIMLR for the inputs defined as described, `nmi` = normalized mutual information as a measure of the inferred clusters compared to the true labels

Source

Zeisel, Amit, et al. "Cell types in the mouse cortex and hippocampus revealed by single-cell RNA-seq." *Science* 347.6226 (2015): 1138-1142.

Index

BuettnerFlorian, [2](#)

SIMLR, [3](#)

SIMLR_Estimate_Number_of_Clusters, [4](#)

SIMLR_Feature_Ranking, [4](#)

SIMLR_Large_Scale, [5](#)

ZeiselAmit, [6](#)