# Package 'scmap'

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Type Package

Title A tool for unsupervised projection of single cell RNA-seq data

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version 1.7.1

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Description Single-cell RNA-seq (scRNA-seq) is widely used to investigate the composition of complex tissues since the technology allows researchers to define cell-types using unsupervised clustering of the transcriptome. However, due to differences in experimental methods and computational analyses, it is often challenging to directly compare the cells identified in two different experiments. scmap is a method for projecting cells from a scRNA-seq experiment on to the cell-types or individual cells identified in a different experiment.

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**Imports** Biobase, SingleCellExperiment, SummarizedExperiment, BiocGenerics, S4Vectors, dplyr, reshape2, matrixStats, proxy, utils, googleVis, ggplot2, methods, stats, e1071, randomForest, Rcpp (>= 0.12.12)

**Depends** R(>= 3.4)

LinkingTo Rcpp, RcppArmadillo

**Encoding UTF-8** 

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Suggests knitr, rmarkdown

VignetteBuilder knitr

biocViews ImmunoOncology, SingleCell, Software, Classification, SupportVectorMachine, RNASeq, Visualization, Transcriptomics, DataRepresentation, Transcription, Sequencing, Preprocessing, GeneExpression, DataImport

NeedsCompilation no

URL https://github.com/hemberg-lab/scmap

BugReports https://support.bioconductor.org/t/scmap/

git\_url https://git.bioconductor.org/packages/scmap

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# R topics documented:

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# Description

Cell type annotations for data extracted from a publication by Yan et al.

# Usage

ann

# **Format**

An object of class data.frame with 90 rows and 1 columns.

## Source

```
http://dx.doi.org/10.1038/nsmb.2660
```

Each row corresponds to a single cell from 'yan' dataset

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and the whole result is returned as a vector. Used as part of the approx. calculations of the cosine similarity between the query and the reference.	EuclSqNorm	prox. calculations of the cosine similarity between the query and the
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#### **Description**

The Euclidean Squared Norm of each column of a matrix is computed and the whole result is returned as a vector. Used as part of the approx. calculations of the cosine similarity between the query and the reference.

# Usage

```
EuclSqNorm(dat)
```

## Arguments

dat A numerical matrix

getSankey	Plot Sankey diagram comparing two clusterings
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### **Description**

Sometimes it is useful to see how the clusters in two different clustering solutions correspond to each other. Sankey diagram is a good way to visualize them. This function takes as input two clustering solutions and visualizes them using a Sankey diagram. The order of the reference clusters is defined by their labels in increasing order.

#### Usage

```
getSankey(reference, clusters, plot_width = 400, plot_height = 600,
  colors = NULL)
```

# Arguments

reference reference clustering labels

clusters clustering labels under investigations

plot\_width width of the output plot in pixels

plot\_height height of the output plot in pixels

colors colors of the links between two clusterings. If defined please note that each cluster in the reference clustering has to have its own color. This should be a normal text vector, e.g. c('#FF0000', '#FFA500', '#008000')

#### Value

```
an object returned by 'gvisSankey'
```

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#### **Examples**

```
plot(getSankey(ann[ , 1], ann[ , 1]))
```

indexCell

Create an index for a dataset to enable fast approximate nearest neighbour search

#### **Description**

The method is based on product quantization for the cosine distance. Split the training data into M identically sized chunks by genes. Use k-means to find k subcentroids for each group. Assign cluster numbers to each member of the dataset.

#### Usage

```
indexCell(object = NULL, M = NULL, k = NULL)
indexCell.SingleCellExperiment(object, M, k)

## S4 method for signature 'SingleCellExperiment'
indexCell(object = NULL, M = NULL,
    k = NULL)
```

#### **Arguments**

object an object of SingleCellExperiment class

M number of chunks into which the expr matrix is split
k number of clusters per group for k-means clustering

#### Value

a list of four objects: 1) a list of matrices containing the subcentroids of each group 2) a matrix containing the subclusters for each cell for each group 3) the value of M 4) the value of k

```
library(SingleCellExperiment)
sce <- SingleCellExperiment(assays = list(normcounts = as.matrix(yan)), colData = ann)
# this is needed to calculate dropout rate for feature selection
# important: normcounts have the same zeros as raw counts (fpkm)
counts(sce) <- normcounts(sce)
logcounts(sce) <- log2(normcounts(sce) + 1)
# use gene names as feature symbols
rowData(sce)$feature_symbol <- rownames(sce)
isSpike(sce, 'ERCC') <- grepl('^ERCC-', rownames(sce))
# remove features with duplicated names
sce <- sce[!duplicated(rownames(sce)), ]
sce <- selectFeatures(sce)
sce <- indexCell(sce)</pre>
```

indexCluster 5

i	ndev()	lister

Create a precomputed Reference

# **Description**

Calculates centroids of each cell type and merge them into a single table.

#### Usage

```
indexCluster(object = NULL, cluster_col = "cell_type1")
indexCluster.SingleCellExperiment(object, cluster_col)
## S4 method for signature 'SingleCellExperiment'
indexCluster(object = NULL,
    cluster_col = "cell_type1")
```

## **Arguments**

object SingleCellExperiment object

cluster\_col column name in the 'colData' slot of the SingleCellExperiment object contain-

ing the cell classification information

#### Value

a 'data.frame' containing calculated centroids of the cell types of the Reference dataset

```
library(SingleCellExperiment)
sce <- SingleCellExperiment(assays = list(normcounts = as.matrix(yan)), colData = ann)
# this is needed to calculate dropout rate for feature selection
# important: normcounts have the same zeros as raw counts (fpkm)
counts(sce) <- normcounts(sce)
logcounts(sce) <- log2(normcounts(sce) + 1)
# use gene names as feature symbols
rowData(sce)$feature_symbol <- rownames(sce)
isSpike(sce, 'ERCC') <- grep1('^ERCC-', rownames(sce))
# remove features with duplicated names
sce <- sce[!duplicated(rownames(sce)), ]
sce <- selectFeatures(sce)
sce <- indexCluster(sce[rowData(sce)$scmap_features, ])</pre>
```

6 normalise

NN	Main nearest neighbour calculation function. Used on the first reference dataset. Returns a list of three objects: 1) the cell indices of the
	w nearest neighbours 2) the corresponding approx. cosine similarities

# Description

Main nearest neighbour calculation function. Used on the first reference dataset. Returns a list of three objects: 1) the cell indices of the w nearest neighbours 2) the corresponding approx. cosine similarities

# Usage

```
NN(w, k, subcentroids, subclusters, query_chunks, M, SqNorm)
```

# Arguments

	And independent of the second
W	An integer specifying the number of nearest neighbours
k	An integer specifying the number of subcentroids for each product quantization chunk
subcentroids	A list of matrices containing the subcentroids of each chunk.
subclusters	A matrix containing the subcentroid assignments of each reference cell. See $scf\_index$ .
query_chunks	A list of matrices containing the chunks of the query dataset after it has been split according to the product quantization method
М	An integer specifying the number of chunks
SqNorm	A numerical vector containing the Euclidean Squared Norm of each query cell.

normalise	Normalises each column of a matrix	

# Description

Normalises each column of a matrix

# Usage

normalise(dat)

# **Arguments**

dat A numerical matrix

scmapCell 7

scmapCell	For each cell in a query dataset, we search for the nearest neighbours
	by cosine distance within a collection of reference datasets.

# Description

For each cell in a query dataset, we search for the nearest neighbours by cosine distance within a collection of reference datasets.

#### Usage

```
scmapCell(projection = NULL, index_list = NULL, w = 10)
scmapCell.SingleCellExperiment(projection, index_list, w)
## S4 method for signature 'SingleCellExperiment'
scmapCell(projection = NULL,
   index_list = NULL, w = 10)
```

#### **Arguments**

```
projection an object of SingleCellExperiment class
index_list list of index objects each coming from the output of 'indexCell'
w a positive integer specifying the number of nearest neighbours to find
```

#### Value

a list of 3 objects: 1) a matrix with the closest w neighbours by cell number of each query cell stored by column 2) a matrix of integers giving the reference datasets from which the above cells came from 3) a matrix with the cosine similarities corresponding to each of the nearest neighbours

```
library(SingleCellExperiment)
sce <- SingleCellExperiment(assays = list(normcounts = as.matrix(yan)), colData = ann)
# this is needed to calculate dropout rate for feature selection
# important: normcounts have the same zeros as raw counts (fpkm)
counts(sce) <- normcounts(sce)
logcounts(sce) <- log2(normcounts(sce) + 1)
# use gene names as feature symbols
rowData(sce)$feature_symbol <- rownames(sce)
isSpike(sce, 'ERCC') <- grepl('^ERCC-', rownames(sce))
# remove features with duplicated names
sce <- sce[!duplicated(rownames(sce)), ]
sce <- selectFeatures(sce)
sce <- indexCell(sce)
scmapCell_results <- scmapCell(sce, list(metadata(sce)$scmap_cell_index))</pre>
```

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scmapCell2Cluster

Approximate k-NN cell-type classification using scfinemap

#### **Description**

Each cell in the query dataset is assigned a cell-type if the similarity between its nearest neighbour exceeds a threshold AND its w nearest neighbours have the same cell-type.

#### Usage

```
scmapCell2Cluster(scmapCell_results = NULL, cluster_list = NULL, w = 3,
    threshold = 0.5)
scmapCell2Cluster.SingleCellExperiment(scmapCell_results, cluster_list, w,
    threshold)
## S4 method for signature 'list'
scmapCell2Cluster(scmapCell_results = NULL,
    cluster_list = NULL, w = 3, threshold = 0.5)
```

### **Arguments**

scmapCell\_results

the output of 'scmapCell()' with 'projection' as its input.

cluster\_list list of cell cluster labels correspondint to each index against which the 'projec-

tion' has been projected

w an integer specifying the number of nearest neighbours to find

threshold the threshold which the maximum similarity between the query and a reference

cell must exceed for the cell-type to be assigned

#### Value

The query dataset with the predicted labels attached to colData(query\_dat)\$cell\_type1

```
library(SingleCellExperiment)
sce <- SingleCellExperiment(assays = list(normcounts = as.matrix(yan)), colData = ann)
# this is needed to calculate dropout rate for feature selection
# important: normcounts have the same zeros as raw counts (fpkm)
counts(sce) <- normcounts(sce)
logcounts(sce) <- log2(normcounts(sce) + 1)
# use gene names as feature symbols
rowData(sce)$feature_symbol <- rownames(sce)
isSpike(sce, 'ERCC') <- grepl('^ERCC-', rownames(sce))
# remove features with duplicated names
sce <- sce[!duplicated(rownames(sce)), ]
sce <- selectFeatures(sce)
sce <- indexCell(sce)
scmapCell_results <- scmapCell(sce, list(metadata(sce)$scmap_cell_index))
sce <- scmapCell2Cluster(scmapCell_results, cluster_list = list(colData(sce)$cell_type1))</pre>
```

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#### **Description**

Projection of one dataset to another

#### Usage

```
scmapCluster(projection = NULL, index_list = NULL, threshold = 0.7)
scmapCluster.SingleCellExperiment(projection, index_list, threshold)
## S4 method for signature 'SingleCellExperiment'
scmapCluster(projection = NULL,
  index_list = NULL, threshold = 0.7)
```

### **Arguments**

projection 'SingleCellExperiment' object to project
index\_list list of index objects each coming from the output of 'indexCluster'
threshold threshold on similarity (or probability for SVM and RF)

#### Value

The projection object of SingleCellExperiment class with labels calculated by 'scmap' and stored in the scmap\_labels column of the rowData(object) slot.

```
library(SingleCellExperiment)
sce <- SingleCellExperiment(assays = list(normcounts = as.matrix(yan)), colData = ann)
# this is needed to calculate dropout rate for feature selection
# important: normcounts have the same zeros as raw counts (fpkm)
counts(sce) <- normcounts(sce)
logcounts(sce) <- log2(normcounts(sce) + 1)
# use gene names as feature symbols
rowData(sce)$feature_symbol <- rownames(sce)
isSpike(sce, 'ERCC') <- grepl('^ERCC-', rownames(sce))
# remove features with duplicated names
sce <- sce[!duplicated(rownames(sce)), ]
sce <- selectFeatures(sce)
sce <- indexCluster(sce)
sce <- scmapCluster(sce, list(metadata(sce)$scmap_cluster_index))</pre>
```

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selectFeatures

Find the most informative features (genes/transcripts) for projection

#### **Description**

This is a modification of the M3Drop method. Instead of fitting a Michaelis-Menten model to the log expression-dropout relation, we fit a linear model. Namely, the linear model is build on the log(expression) versus log(dropout) distribution. After fitting a linear model important features are selected as the top N residuals of the linear model.

#### Usage

```
selectFeatures(object, n_features = 500, suppress_plot = TRUE)
selectFeatures.SingleCellExperiment(object, n_features, suppress_plot)
## S4 method for signature 'SingleCellExperiment'
selectFeatures(object, n_features = 500,
    suppress_plot = TRUE)
```

#### **Arguments**

object an object of SingleCellExperiment class n\_features number of the features to be selected

 $suppress\_plot \quad boolean \ parameter, which \ defines \ whether \ to \ plot \ log(expression) \ versus \ log(dropout)$ 

distribution for all genes. Selected features are highlighted with the red colour.

# Details

Please note that feature\_symbol column of rowData(object) must be present in the input object and should not contain any duplicated feature names. This column defines feature names used during projection. Feature symbols in the reference dataset must correpond to the feature symbols in the projection dataset, otherwise the mapping will not work!

#### Value

an object of SingleCellExperiment class with a new column in rowData(object) slot which is called scmap\_features. It can be accessed by using as.data.frame(rowData(object))\$scmap\_features.

```
library(SingleCellExperiment)
sce <- SingleCellExperiment(assays = list(normcounts = as.matrix(yan)), colData = ann)
# this is needed to calculate dropout rate for feature selection
# important: normcounts have the same zeros as raw counts (fpkm)
counts(sce) <- normcounts(sce)
logcounts(sce) <- log2(normcounts(sce) + 1)
# use gene names as feature symbols
rowData(sce)$feature_symbol <- rownames(sce)
isSpike(sce, 'ERCC') <- grepl('^ERCC-', rownames(sce))
# remove features with duplicated names
sce <- sce[!duplicated(rownames(sce)), ]</pre>
```

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```
sce <- selectFeatures(sce)</pre>
```

setFeatures

Set the most important features (genes/transcripts) for projection

## **Description**

This method manually sets the features to be used for projection.

#### Usage

```
setFeatures(object, features = NULL)
setFeatures.SingleCellExperiment(object, features)
## S4 method for signature 'SingleCellExperiment'
setFeatures(object, features = NULL)
```

## **Arguments**

object an object of SingleCellExperiment class

features a character vector of feature names

#### **Details**

Please note that feature\_symbol column of rowData(object) must be present in the input object and should not contain any duplicated feature names. This column defines feature names used during projection. Feature symbols in the reference dataset must correpond to the feature symbols in the projection dataset, otherwise the mapping will not work!

## Value

an object of SingleCellExperiment class with a new column in rowData(object) slot which is called scmap\_features. It can be accessed by using as.data.frame(rowData(object))\$scmap\_features.

```
library(SingleCellExperiment)
sce <- SingleCellExperiment(assays = list(normcounts = as.matrix(yan)), colData = ann)
# this is needed to calculate dropout rate for feature selection
# important: normcounts have the same zeros as raw counts (fpkm)
counts(sce) <- normcounts(sce)
logcounts(sce) <- log2(normcounts(sce) + 1)
# use gene names as feature symbols
rowData(sce)$feature_symbol <- rownames(sce)
isSpike(sce, 'ERCC') <- grepl('^ERCC-', rownames(sce))
# remove features with duplicated names
sce <- sce[!duplicated(rownames(sce)), ]
sce <- setFeatures(sce, c('MMP2', 'ZHX3'))</pre>
```

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subdistsmult	Computes the dot product between the subcentroids from the indexed reference and the subvectors of an element of the query dataset. Returns an M by k matrix. Used as an intermediate step (in NNfirst and NNmult) for calculating an approximation of the cosine similarity between the query and the reference.
	The state of the s

# Description

Computes the dot product between the subcentroids from the indexed reference and the subvectors of an element of the query dataset. Returns an M by k matrix. Used as an intermediate step (in NNfirst and NNmult) for calculating an approximation of the cosine similarity between the query and the reference.

# Usage

```
subdistsmult(subcentroids, query_chunks, M, k, cellnum)
```

#### **Arguments**

S	
subcentroids	A list of matrices containing the subcentroids of each chunk.
query_chunks	A list of matrices containing the chunks of the query dataset after it has been split according to the product quantization method
М	An integer specifying the number of chunks
k	An integer specifying the number of subcentroids per chunk
cellnum	An integer specifying the column of the query dataset we wish to consider

yan	Single cell RNA-Seq data extracted from a publication by Yan et al.

# Description

Single cell RNA-Seq data extracted from a publication by Yan et al.

## Usage

yan

## **Format**

An object of class data. frame with 20214 rows and 90 columns.

#### Source

```
http://dx.doi.org/10.1038/nsmb.2660
```

Columns represent cells, rows represent genes expression values.

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