Package 'sketchR'

November 12, 2026

Version 1.8.0

Date 2026-04-02

Title An R interface for python subsampling/sketching algorithms

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Description Provides an R interface for various subsampling algorithms implemented in python packages. Currently, interfaces to the geosketch and scSampler python packages are implemented. In addition it also provides diagnostic plots to evaluate the subsampling.

Imports basilisk, Biobase, DelayedArray, dplyr, ggplot2, methods, reticulate, rlang, scales, stats

Suggests rmarkdown, knitr, testthat (>= 3.0.0), TENxPBMCData, scuttle, scran, scater, SingleR, celldex, cowplot, SummarizedExperiment, beachmat.hdf5, BiocStyle, BiocManager, SingleCellExperiment, snifter, uwot, bluster, class

URL https://github.com/fmicompbio/sketchR

BugReports https://github.com/fmicompbio/sketchR/issues

RoxygenNote 7.3.3

Encoding UTF-8

StagedInstall no

Config/testthat/edition 3

VignetteBuilder knitr

biocViews SingleCell

git_url https://git.bioconductor.org/packages/sketchR

git_branch RELEASE_3_23

git_last_commit 55176fc

git_last_commit_date 2026-04-28

Repository Bioconductor 3.23

Date/Publication 2026-11-11

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`sketchR-package` *sketchR - an R interface for python subsampling/sketching algorithms*

Description

The sketchR package provides an R interface for various subsampling algorithms implemented in python packages. Currently, interfaces to the geosketch and scSampler python packages are implemented, in the functions geosketch() and scsampler(), respectively. In addition the package also provides diagnostic plots to evaluate the subsampling. More details on how to get started and incorporate the subsampling into an scRNA-seq workflow are provided in the vignette.

Author(s)

Charlotte Soneson

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See Also

Useful links:

- https://github.com/fmicompbio/sketchR
- Report bugs at https://github.com/fmicompbio/sketchR/issues

compareCompositionPlot *Compare the compositions of a data set and a subset*

Description

Plot the composition of a data set (e.g., the number of cells from each cell type) and contrast it with the corresponding composition of a subset.

Usage

```
compareCompositionPlot(
  df,
  idx,
  column,
  showPercentages = TRUE,
  fontSizePercentages = 4
)
```

Arguments

df	A data.frame-like object (such that df[[column]] works).
idx	A numeric vector representing the row indexes of df corresponding to the subset of interest. Can also be a named list of index vectors if multiple subsets are of interest.
column	A character scalar corresponding to a column of df and representing the variable for which the composition should be calculated.
showPercentages	Logical scalar, indicating whether relative frequencies of each category should be shown in the plot.
fontSizePercentages	Numerical scalar, indicating the font size of the relative frequencies, if showPercentages is TRUE.

Value

A ggplot object.

Author(s)

Charlotte Soneson

Examples

```
df <- data.frame(celltype = sample(LETTERS[1:5], 1000, replace = TRUE,
                                   prob = c(0.1, 0.2, 0.5, 0.05, 0.15)))
idx <- sample(seq_len(1000), 200)
compareCompositionPlot(df, idx, "celltype")
```

---

geosketch *Run geosketch to subsample a matrix*

Description

Perform geometric sketching with the geosketch python package.

Usage

```
geosketch(
  mat,
  N,
  replace = FALSE,
  k = "auto",
  alpha = 0.1,
  seed = NULL,
  max_iter = 200,
  one_indexed = TRUE,
  verbose = FALSE
)
```

Arguments

mat	m x n matrix. Samples (the dimension along which to subsample) should be in the rows, features in the columns.
N	Numeric scalar, the number of samples to retain.
replace	Logical scalar, whether to sample with replacement.
k	Numeric scalar or "auto", specifying the number of covering. If k = "auto" (the default), it is set to sqrt(nrow(mat)) for replace = TRUE and to N for replace = FALSE.
alpha	Numeric scalar defining the acceptable interval around k. Binary search halts when it obtains between k * (1 - alpha) and k * (1 + alpha) covering boxes.
seed	Numeric scalar or NULL (default). If not NULL, it will be converted to integer and passed to numpy to seed the random number generator.
max_iter	Numeric scalar giving the maximum iterations at which to terminate binary search in rare cases of non-monotonicity of covering boxes.
one_indexed	Logical scalar, whether to return one-indexed indices.
verbose	Locigal scalar, whether to print logging output while running.

Details

The first time this function is run, it will create a conda environment containing the `geosketch` package. This is done via the `basilisk` R/Bioconductor package - see the documentation for that package for troubleshooting.

Value

A numeric vector with indices to retain.

Author(s)

Charlotte Soneson, Michael Stadler

References

Hie et al (2019): Geometric sketching compactly summarizes the single-cell transcriptomic landscape. Cell Systems 8, 483–493.

Examples

```
x <- matrix(rnorm(500), nrow = 100)
geosketch(mat = x, N = 10, seed = 42)
```

`getGeosketchNames` *Get names of geosketch functions*

Description

Get names of geosketch functions

Usage

```
getGeosketchNames()
```

Value

A list of names of objects exposed in the geosketch module

Author(s)

Charlotte Soneson

Examples

```
getGeosketchNames()
```

getScSamplerNames *Get names of scSampler functions*

Description

Get names of scSampler functions

Usage

```
getScSamplerNames()
```

Value

A list of names of objects exposed in the scSampler module

Author(s)

Charlotte Soneson

Examples

```
if (!(Sys.info()["sysname"] == "Darwin" && Sys.info()["machine"] == "arm64")) {
    getScSamplerNames()
}
```

hausdorffDistPlot *Create diagnostic plot of Hausdorff distances*

Description

Create diagnostic plot showing the Hausdorff distance between a sketch and the full data set, for varying sketch sizes. For reproducibility, seed the random number generator before calling this function using `set.seed`.

Usage

```
hausdorffDistPlot(
  mat,
  Nvec,
  Nrep = 5,
  q = 1e-04,
  methods = c("geosketch", "scsampler", "uniform"),
  extraArgs = list()
)
```

Arguments

mat	m x n matrix. Samples (the dimension along which to subsample) should be in the rows, features in the columns.
Nvec	Numeric vector of sketch sizes.
Nrep	Numeric scalar indicating the number of sketches to draw for each sketch size.
q	Numeric scalar in [0,1], indicating the fraction of largest minimum distances to discard when calculating the robust Hausdorff distance. Setting q=0 gives the classical Hausdorff distance. The default is 1e-4, as suggested by Hie et al (2019).
methods	Character vector, indicating which method(s) to include in the plot. Should be a subset of c("geosketch", "scsampler", "uniform"), where "uniform" randomly samples from input features with uniform probabilities.
extraArgs	Named list providing extra arguments to the respective methods (beyond the matrix and the sketch size). The names of the list should be the method names (currently, "geosketch" or "scsampler"), and each list element should be a named list of argument values. See the examples for an illustration of how to use this argument. Note that the seed argument, if provided to any of the methods, will be ignored (since it would imply providing the same seed for each repeated run of the sketching).

Value

A ggplot object.

Author(s)

Charlotte Soneson, Michael Stadler

References

Hie et al (2019): Geometric sketching compactly summarizes the single-cell transcriptomic landscape. Cell Systems 8, 483–493.

Song et al (2022): scSampler: fast diversity-preserving subsampling of large-scale single-cell transcriptomic data. bioRxiv doi:10.1101/2022.01.15.476407

Huttenlocher et al (1993): Comparing images using the Hausdorff distance. IEEE Transactions on Pattern Analysis and Machine Intelligence 15(9), 850-863.

Examples

```
## Generate example data matrix
mat <- matrix(rnorm(1000), nrow = 100)

## Generate diagnostic Hausdorff distance plot
hausdorffDistPlot(mat, Nvec = c(10, 25, 50),
                  methods = c("geosketch", "uniform"))

## Provide additional arguments for geosketch
```

```
hausdorffDistPlot(mat, Nvec = c(10, 25, 50), Nrep = 2,
                  methods = c("geosketch", "uniform"),
                  extraArgs = list(geosketch = list(max_iter = 100)))
```

`scsampler` *Run scSampler to subsample a matrix*

Description

Perform subsampling with the `scSampler` python package.

Usage

```
scsampler(mat, N, random_split = 1, seed = 0)
```

Arguments

`mat`	m x n matrix. Samples (the dimension along which to subsample) should be in the rows, features in the columns.
`N`	Numeric scalar, the number of samples to retain.
`random_split`	Numeric scalar, the number of parts to randomly split the data into before subsampling within each part. A larger value will speed up computations, but give less optimal results.
`seed`	Numeric scalar, passed to `scsampler` to seed the random number generator.

Details

The first time this function is run, it will create a conda environment containing the `scSampler` package. This is done via the `basilisk` R/Bioconductor package - see the documentation for that package for troubleshooting.

Value

A numeric vector with indices to retain.

Author(s)

Charlotte Soneson, Michael Stadler

References

Song et al (2022): scSampler: fast diversity-preserving subsampling of large-scale single-cell transcriptomic data. bioRxiv doi:10.1101/2022.01.15.476407

Examples

```
if (!(Sys.info()["sysname"] == "Darwin" && Sys.info()["machine"] == "arm64")) {
    x <- matrix(rnorm(500), nrow = 100)
    scsampler(mat = x, N = 10)
}
```

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