

Package ‘zellkonverter’

March 30, 2021

Title Conversion Between scRNA-seq Objects

Version 1.0.3

Date 2021-03-08

Description Provides methods to convert between Python AnnData objects and SingleCellExperiment objects. These are primarily intended for use by downstream Bioconductor packages that wrap Python methods for single-cell data analysis. It also includes functions to read and write H5AD files used for saving AnnData objects to disk.

biocViews SingleCell, DataImport, DataRepresentation

License MIT + file LICENSE

Imports Matrix, basilisk, reticulate, SingleCellExperiment (>= 1.11.6), SummarizedExperiment, DelayedArray, methods, S4Vectors, utils

Suggests covr, spelling, testthat, knitr, rmarkdown, BiocStyle, scRNAseq, HDF5Array, rhdf5

URL <https://github.com/theislab/zellkonverter>

BugReports <https://github.com/theislab/zellkonverter/issues>

Encoding UTF-8

LazyData true

Roxygen list(markdown = TRUE)

RoxygenNote 7.1.1

Language en-GB

StagedInstall no

VignetteBuilder knitr

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

git_branch RELEASE_3_12

git_last_commit e504d10

git_last_commit_date 2021-03-08

Date/Publication 2021-03-29

Author Luke Zappia [aut, cre] (<<https://orcid.org/0000-0001-7744-8565>>),
Aaron Lun [aut] (<<https://orcid.org/0000-0002-3564-4813>>)

Maintainer Luke Zappia <luke@lazappi.id.au>

R topics documented:

zellkonverter-package	2
AnnData-Conversion	2
AnnDataDependencies	4
readH5AD	5
writeH5AD	6
Index	8

zellkonverter-package *zellkonverter: Conversion Between scRNA-seq Objects*

Description

Provides methods to convert between Python AnnData objects and SingleCellExperiment objects. These are primarily intended for use by downstream Bioconductor packages that wrap Python methods for single-cell data analysis. It also includes functions to read and write H5AD files used for saving AnnData objects to disk.

Author(s)

Maintainer: Luke Zappia <luke@lazappi.id.au> ([ORCID](#))

Authors:

- Aaron Lun <infinite.monkeys.with.keyboards@gmail.com> ([ORCID](#))

See Also

Useful links:

- <https://github.com/theislab/zellkonverter>
- Report bugs at <https://github.com/theislab/zellkonverter/issues>

AnnData-Conversion *Convert AnnData between and SingleCellExperiment*

Description

Conversion between Python AnnData objects and [SingleCellExperiment](#) objects.

Usage

```
AnnData2SCE(adata, skip_assays = FALSE, hdf5_backed = TRUE)
```

```
SCE2AnnData(sce, X_name = NULL, skip_assays = FALSE)
```

Arguments

adata	A reticulate reference to a Python AnnData object.
skip_assays	Logical scalar indicating whether to skip conversion of any assays in sce or adata, replacing them with empty sparse matrices instead.
hdf5_backed	Logical scalar indicating whether HDF5-backed matrices in adata should be represented as HDF5Array objects. This assumes that adata is created with backed="r".
sce	A SingleCellExperiment object.
X_name	Name of the assay to use as the primary matrix (X) of the AnnData object. If NULL, the first assay of sce will be used by default.

Details

These functions assume that an appropriate Python environment has already been loaded. As such, they are largely intended for developer use, most typically inside a **basilisk** context.

The conversion is not entirely lossless. The current mapping is shown below (also at <https://tinyurl.com/AnnData2SCE>):

SingleCellExperiment			AnnData			
R object used by Bioconductor packages			Python object used by Scanpy and related packages			
Rows contain features and columns contain cells			Rows contain observations (cells) and columns contain variables (features)			
IMPLEMENTED	Each element is a matrix of expression values with the same dimensions	SimpleList of matrices	assays	X	Numpy array	Primary matrix of expression data
	Any unstructured data	list	metadata	layers	Dictionary of arrays	Dictionary-like object where each element is an array of expression values with the same dimensions as X
	Names of rows (cells)	vector	colnames	uns	OrderedDict	Unstructured annotation
	Columns describe annotations of the columns (cells)	DataFrame	colData	obs_names	Pandas index	Names of observations (cells)
	Each element is a matrix where the number of rows is equal to the number of cells and each column is a dimension	List of matrices	reducedDims	obs	Pandas DataFrame	One-dimensional annotations of the observations (cells)
	Relationships between columns (cells)	List of SelfHits	colPairs	obsm	Dictionary of arrays	Dictionary-like object where each element is an array where the number of rows is equal to the number of observations (cells)
	Relationships between columns (cells)	List of SelfHits	colPairs	obsp	Dictionary of arrays	Dictionary-like object where each element is a square array containing annotations between observations (cells)
	Names of rows (features)	vector	rownames	var_names	Pandas index	Names of variables (features)
	Columns describe annotations of the rows (features)	DataFrame	rowData	vars	Pandas DataFrame	One-dimensional annotations of the variables (features)
	Relationships between rows (features)	List of SelfHits	rowPairs	varm	Dictionary of arrays	Dictionary-like object where each element is an array where the number of rows is equal to the number of variables (features)
NOT IMPLEMENTED	Nested SingleCellExperiments with information about alternative feature sets	List of SingleCellExperiments	altExp	varp	Dictionary of arrays	Dictionary-like object where each element is a square array containing annotations between variables (features)
	Internal unstructured data that is not meant to be modified by users	list	int_metadata	raw	AnnData	Raw version of X and var prior to any filtering. Is not indexed as part of the object.
	Internal annotation for columns (cells) that is not meant to be modified by users	DataFrame	int_colData			
	Internal annotation for rows (features) that is not meant to be modified by users	DataFrame	int_elementMetadata			

In `SCE2AnnData()`, matrices are converted to a **numpy**-friendly format. Sparse matrices are converted to `dgCMMatrix` objects while all other matrices are converted into ordinary matrices. If `skip_assays = TRUE`, empty sparse matrices are created instead and the user is expected to fill in the assays on the Python side.

For `AnnData2SCE()`, a warning is raised if there is no corresponding R format for a matrix in the AnnData object, and an empty sparse matrix is created instead as a placeholder. If `skip_assays = NA`, no warning is emitted but variables are created in the `int_metadata()` of the output to specify which assays were skipped. If `skip_assays = TRUE`, empty sparse matrices are created for all assays, regardless of whether they might be convertible to an R format or not. In both cases, the user is expected to fill in the assays on the R side, see `readH5AD()` for an example.

We attempt to convert between items in the `SingleCellExperiment metadata()` slot and the AnnData `uns` slot. If an item cannot be converted a warning will be raised.

Values stored in the `varm` slot of an AnnData object are stored in a column of `rowData()` in a `SingleCellExperiment` as a `DataFrame` of matrices. No attempt is made to transfer this information when converting from `SingleCellExperiment` to AnnData.

Value

AnnData2SCE() will return a [SingleCellExperiment](#) containing the equivalent data from adata.

SCE2AnnData() will return a **reticulate** reference to an AnnData object containing the content of sce.

Author(s)

Luke Zappia

Aaron Lun

See Also

[writeH5AD\(\)](#) and [readH5AD\(\)](#) for dealing directly with H5AD files.

Examples

```
if (requireNamespace("scRNAseq", quietly = TRUE)) {
  library(basilisk)
  library(scRNAseq)
  seger <- SegerstolpePancreasData()

  # These functions are designed to be run inside
  # a specified Python environment
  roundtrip <- basiliskRun(fun = function(sce) {
    # Convert SCE to AnnData:
    adata <- SCE2AnnData(sce)

    # Maybe do some work in Python on 'adata':
    # BLAH BLAH BLAH

    # Convert back to an SCE:
    AnnData2SCE(adata)
  }, env = zellkonverter:::anndata_env, sce = seger)
}
```

AnnDataDependencies *AnnData dependencies*

Description

Vector defining a set of Python dependencies and versions required to operate with AnnData and H5AD files.

Usage

```
.AnnDataDependencies
```

Format

A character vector containing the pinned versions of all Python packages on which AnnData depends.

Details

This variable is exposed for use by other package developers who want an easy way to define the dependencies required for creating a Python environment to work with AnnData objects, most typically within a **basilisk** context. For example, we can simply combine this vector with additional dependencies to create a **basilisk** environment with Python package versions that are consistent with those in **zellkonverter**.

Author(s)

Luke Zappia
Aaron Lun

Examples

```
.AnnDataDependencies
```

readH5AD

Read H5AD

Description

Reads a H5AD file and returns a [SingleCellExperiment](#) object.

Usage

```
readH5AD(file, use_hdf5 = FALSE)
```

Arguments

<code>file</code>	String containing a path to a .h5ad file.
<code>use_hdf5</code>	Logical scalar indicating whether assays should be loaded as HDF5-based matrices from the HDF5Array package.

Details

Setting `use_hdf5 = TRUE` allows for very large datasets to be efficiently represented on machines with little memory. However, this comes at the cost of access speed as data needs to be fetched from the HDF5 file upon request.

When first run, this function will instantiate a conda environment containing all of the necessary dependencies. This will not be performed on any subsequent run or if any other **zellkonverter** function has been run prior to this one.

Value

A [SingleCellExperiment](#) object is returned.

Author(s)

Luke Zappia
Aaron Lun

See Also

`writeH5AD()`, to write a [SingleCellExperiment](#) object to a H5AD file.

`AnnData2SCE()`, for developers to convert existing `AnnData` instances to a [SingleCellExperiment](#).

Examples

```
library(SummarizedExperiment)

file <- system.file("extdata", "krumsiek11.h5ad", package = "zellkonverter")
sce <- readH5AD(file)
class(assay(sce))

sce2 <- readH5AD(file, use_hdf5 = TRUE)
class(assay(sce2))
```

writeH5AD

Write H5AD

Description

Write a H5AD file from a [SingleCellExperiment](#) object.

Usage

```
writeH5AD(sce, file, X_name = NULL, skip_assays = FALSE)
```

Arguments

<code>sce</code>	A SingleCellExperiment object.
<code>file</code>	String containing a path to write the new <code>.h5ad</code> file.
<code>X_name</code>	Name of the assay to use as the primary matrix (X) of the <code>AnnData</code> object. If <code>NULL</code> , the first assay of <code>sce</code> will be used by default.
<code>skip_assays</code>	Logical scalar indicating whether assay matrices should be ignored when writing to file.

Details

Setting `skip_assays=TRUE` can occasionally be useful if the matrices in `sce` are stored in a format that is not amenable for efficient conversion to a **numpy**-compatible format. In such cases, it can be better to create an empty placeholder dataset in `file` and fill it in R afterwards.

When first run, this function will instantiate a conda environment containing all of the necessary dependencies. This will not be performed on any subsequent run or if any other **zellkonverter** function has been run prior to this one.

The **anndata** package automatically converts some character vectors to factors when saving `.h5ad` files. This can effect columns of `rowData(sce)` and `colData(sce)` which may change type when the `.h5ad` file is read back into R.

Value

A `NULL` is invisibly returned.

Author(s)

Luke Zappia
Aaron Lun

See Also

[readH5AD\(\)](#), to read a [SingleCellExperiment](#) file from a H5AD file.
[SCE2AnnData\(\)](#), for developers to create an AnnData object from a [SingleCellExperiment](#).

Examples

```
# Using the Zeisel brain dataset
if (requireNamespace("scRNAseq", quietly = TRUE)) {
  library(scRNAseq)
  sce <- ZeiselBrainData()

  # Writing to a H5AD file
  temp <- tempfile(fileext = ".h5ad")
  writeH5AD(sce, temp)
}
```

Index

* datasets

AnnDataDependencies, 4

.AnnDataDependencies

(AnnDataDependencies), 4

AnnData-Conversion, 2

AnnData2SCE (AnnData-Conversion), 2

AnnData2SCE(), 6

AnnDataDependencies, 4

DataFrame, 3

dgCMatrix, 3

int_metadata(), 3

metadata(), 3

readH5AD, 5

readH5AD(), 3, 4, 7

rowData(), 3

SCE2AnnData (AnnData-Conversion), 2

SCE2AnnData(), 7

SingleCellExperiment, 2-7

writeH5AD, 6

writeH5AD(), 4, 6

zellkonverter (zellkonverter-package), 2

zellkonverter-package, 2