

Package ‘zellkonverter’

November 21, 2023

Title Conversion Between scRNA-seq Objects

Version 1.12.1

Date 2023-11-13

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, cli

Suggests anndata, BiocFileCache, BiocStyle, covr, HDF5Array, knitr, pkgload, rmarkdown, rhdf5 (>= 2.45.1), scRNAseq, spelling, testthat, withr

Collate 'AnnData2SCE.R' 'SCE2AnnData.R' 'ui.R' 'basilisk.R' 'read.R' 'reticulate.R' 'utils.R' 'validation.R' 'write.R' 'zellkonverter-package.R'

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

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

Encoding UTF-8

LazyData true

Roxygen list(markdown = TRUE)

RoxygenNote 7.2.3

Language en-GB

StagedInstall no

VignetteBuilder knitr

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

git_branch RELEASE_3_18

git_last_commit 4cb6fc2

git_last_commit_date 2023-11-13

Repository Bioconductor 3.18

Date/Publication 2023-11-20

Author Luke Zappia [aut, cre] (<<https://orcid.org/0000-0001-7744-8565>>),
 Aaron Lun [aut] (<<https://orcid.org/0000-0002-3564-4813>>),
 Jack Kamm [ctb] (<<https://orcid.org/0000-0003-2412-756X>>),
 Robrecht Cannoodt [ctb] (<<https://orcid.org/0000-0003-3641-729X>>,
 rcannood)

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

R topics documented:

zellkonverter-package	2
AnnData-Conversion	3
AnnData-Environment	6
expectSCE	7
r-py-conversion	8
readH5AD	9
setZellkonverterVerbose	10
validateH5ADSCE	11
writeH5AD	12
Index	15

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](#))

Other contributors:

- Jack Kamm <jackkamm@gmail.com> ([ORCID](#)) [contributor]
- Robrecht Cannoodt <rcannood@gmail.com> ([ORCID](#)) (rcannood) [contributor]

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,  
    X_name = NULL,  
    layers = TRUE,  
    uns = TRUE,  
    var = TRUE,  
    obs = TRUE,  
    varm = TRUE,  
    obsm = TRUE,  
    varp = TRUE,  
    obsp = TRUE,  
    raw = FALSE,  
    skip_assays = FALSE,  
    hdf5_backed = TRUE,  
    verbose = NULL  
)
```

```
SCE2AnnData(  
    sce,  
    X_name = NULL,  
    assays = TRUE,  
    colData = TRUE,  
    rowData = TRUE,  
    varm = TRUE,  
    reducedDims = TRUE,  
    metadata = TRUE,  
    colPairs = TRUE,  
    rowPairs = TRUE,  
    skip_assays = FALSE,  
    verbose = NULL  
)
```

Arguments

adata	A reticulate reference to a Python AnnData object.
X_name	For SCE2AnnData() 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. For AnnData2SCE() name used when saving X as an assay. If NULL looks for an X_name value in uns, otherwise uses "X".
layers, uns, var, obs, varm, obsm, varp, obsp, raw	Arguments specifying how these slots are converted. If TRUE everything in that slot is converted, if FALSE nothing is converted and if a character vector only those items or columns are converted.
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".
verbose	Logical scalar indicating whether to print progress messages. If NULL uses getOption("zellkonverter.verbose").
sce	A SingleCellExperiment object.
assays, colData, rowData, reducedDims, metadata, colPairs, rowPairs	Arguments specifying how these slots are converted. If TRUE everything in that slot is converted, if FALSE nothing is converted and if a character vector only those items or columns are converted.

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)
	Names of rows (features)	vector	rownames	↔	obsp	Dictionary of arrays	Dictionary-like object where each element is a square array containing annotations between observations (cells)
	Columns describe annotations of the rows (features)	DataFrame	rowData	↔	var_names	Pandas index	Names of variables (features)
	Relationships between rows (features)	List of SelfHits	rowPairs	↔	vars	Pandas DataFrame	One-dimensional annotations of the variables (features)
	Nested SingleCellExperiments with information about alternative feature sets	List of SingleCellExperiments	altExp	↔	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	Internal unstructured data that is not meant to be modified by users	list	int_metadata		varp	Dictionary of arrays	Dictionary-like object where each element is a square array containing annotations between variables (features)
	Internal annotation for columns (cells) that is not meant to be modified by users	DataFrame	int_colData		raw	AnnData	Raw version of X and var prior to any filtering. Is not indexed as part of the object.
	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 `dgCMatrix` 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. If this column is present an 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 <- zellkonverter::SCE2AnnData(sce)

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

    # Convert back to an SCE:
```

```

    zellkonverter::AnnData2SCE(adata)
  }, env = zellkonverterAnnDataEnv(), sce = seger)
}

```

AnnData-Environment *AnnData environment*

Description

The Python environment used by **zellkonverter** for interfacing with the **anndata** Python library (and H5AD files) is described by the dependencies in returned by `AnnDataDependencies()`. The `zellkonverterAnnDataEnv()` functions returns the `basilisk::BasiliskEnvironment()` containing these dependencies used by **zellkonverter**. Allowed versions of **anndata** are available in `.AnnDataVersions`.

Usage

```

. AnnDataVersions

AnnDataDependencies(version = .AnnDataVersions)

zellkonverterAnnDataEnv(version = .AnnDataVersions)

```

Arguments

version A string giving the version of the **anndata** Python library to use. Allowed values are available in `.AnnDataVersions`. By default the latest version is used.

Format

For `.AnnDataVersions` a character vector containing allowed **anndata** version strings.

Details

Using Python environments:

When a **zellkonverter** is first run a conda environment containing all of the necessary dependencies for that version will be instantiated. This will not be performed on any subsequent run or if any other **zellkonverter** function has been run prior with the same environment version.

By default the **zellkonverter** conda environment will become the shared R Python environment if one does not already exist. When one does exist (for example when a **zellkonverter** function has already been run using a different environment version) then a separate environment will be used. See `basilisk::setBasiliskShared()` for more information on this behaviour. Note that when the environment is not shared progress messages are lost.

Development:

The `AnnDataDependencies()` function 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**.

If you want to run code in the exact environment used by **zellkonverter** this can be done using `zellkonverterAnnDataEnv()` in combination with `basilisk::basiliskStart()` and/or `basilisk::basiliskRun()`. Please refer to the **basilisk** documentation for more information on using these environments.

Value

For `AnnDataDependencies` a character vector containing the pinned versions of all Python packages to be used by `zellkonverterAnnDataEnv()`.

For `zellkonverterAnnDataEnv` a `basilisk::BasiliskEnvironment()` containing **zellkonverter**'s `AnnData` Python environment.

Author(s)

Luke Zappia

Aaron Lun

Examples

```
.AnnDataVersions

AnnDataDependencies()
AnnDataDependencies(version = "0.7.6")

cl <- basilisk::basiliskStart(zellkonverterAnnDataEnv())
anndata <- reticulate::import("anndata")
basilisk::basiliskStop(cl)
```

expectSCE

Expect SCE

Description

Test that a `SingleCellExperiment` matches an expected object. Designed to be used inside `testthat::test_that()` during package testing.

Usage

```
expectSCE(sce, expected)
```

Arguments

`sce` A `SingleCellExperiment` object.

`expected` A template `SingleCellExperiment` object to compare to.

Value

TRUE invisibly if checks pass

Author(s)

Luke Zappia

r-py-conversion

Convert between Python and R objects

Description

Convert between Python and R objects

Usage

```
## S3 method for class 'numpy.ndarray'  
py_to_r(x)
```

Arguments

x A Python object.

Details

These functions are extensions of the default conversion functions in the `reticulate` package for the following reasons:

- `numpy.ndarray` - Handle conversion of **numpy** recarrays
- `pandas.core.arrays.masked.BaseMaskedArray` - Handle conversion of **pandas** arrays (used when by `AnnData` objects when there are missing values)
- `pandas.core.arrays.categorical.Categorical` - Handle conversion of **pandas** categorical arrays

Value

An R object, as converted from the Python object.

Author(s)

Luke Zappia

See Also

[reticulate::py_to_r\(\)](#) for the base `reticulate` functions

readH5AD	<i>Read H5AD</i>
----------	------------------

Description

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

Usage

```
readH5AD(
  file,
  X_name = NULL,
  use_hdf5 = FALSE,
  reader = c("python", "R"),
  version = NULL,
  verbose = NULL,
  ...
)
```

Arguments

file	String containing a path to a .h5ad file.
X_name	Name used when saving X as an assay. If NULL looks for an X_name value in uns, otherwise uses "X".
use_hdf5	Logical scalar indicating whether assays should be loaded as HDF5-based matrices from the HDF5Array package.
reader	Which HDF5 reader to use. Either "python" for reading with the anndata Python package via reticulate or "R" for zellkonverter 's native R reader.
version	A string giving the version of the anndata Python library to use. Allowed values are available in <code>.AnnDataVersions</code> . By default the latest version is used.
verbose	Logical scalar indicating whether to print progress messages. If NULL uses <code>getOption("zellkonverter.verbose")</code> .
...	Arguments passed on to AnnData2SCE
	layers, uns, var, obs, varm, obsm, varp, obsp, raw Arguments specifying how these slots are converted. If TRUE everything in that slot is converted, if FALSE nothing is converted and if a character vector only those items or columns are converted.
	skip_assays Logical scalar indicating whether to skip conversion of any assays in sce or adata, replacing them with empty sparse matrices instead.

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.

Setting `reader = "R"` will use an experimental native R reader instead of reading the file into Python and converting the result. This avoids the need for a Python environment and some of the issues with conversion but is still under development and is likely to return slightly different output.

See [AnnData-Environment](#) for more details on **zellkonverter** Python environments.

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))

sce3 <- readH5AD(file, reader = "R")
```

setZellkonverterVerbose

Set zellkonverter verbose

Description

Set the zellkonverter verbosity option

Usage

```
setZellkonverterVerbose(verbose = TRUE)
```

Arguments

`verbose` Logical value for the verbosity option.

Details

Running `setZellkonverterVerbose(TRUE)` will turn on **zellkonverter** progress messages by default without having to set `verbose = TRUE` in each function call. This is done by setting the `"zellkonverter.verbose"` option. Running `setZellkonverterVerbose(FALSE)` will turn default verbosity off.

Value

The value of `getOption("zellkonverter.verbose")` invisibly

Examples

```
current <- getOption("zellkonverter.verbose")
setZellkonverterVerbose(TRUE)
getOption("zellkonverter.verbose")
setZellkonverterVerbose(FALSE)
getOption("zellkonverter.verbose")
setZellkonverterVerbose(current)
getOption("zellkonverter.verbose")
```

 validateH5ADSCE

Validate H5AD SCE

Description

Validate a `SingleCellExperiment` created by `readH5AD()`. Designed to be used inside `testthat::test_that()` during package testing.

Usage

```
validateH5ADSCE(sce, names, missing)
```

Arguments

<code>sce</code>	A SingleCellExperiment object.
<code>names</code>	Named list of expected names. Names are slots and values are vectors of names that are expected to exist in that slot.
<code>missing</code>	Named list of known missing names. Names are slots and values are vectors of names that are expected to not exist in that slot.

Details

This function checks that a `SingleCellExperiment` contains the expected items in each slot. The main reason for this function is avoid repeating code when testing multiple `.h5ad` files. The following items in `names` and `missing` are recognised:

- `assays` - Assay names

- colData - colData column names
- rowData - rowData column names
- metadata - metadata names
- redDim - Reduced dimension names
- varm - Column names of the varm rowData column (from the AnnData varm slot)
- colPairs - Column pair names
- rowPairs - rowData pair names
- raw_rowData - rowData columns names in the raw altExp
- raw_varm - Column names of the raw varm rowData column (from the AnnData varm slot)

If an item in names or missing is NULL then it won't be checked. The items in missing are checked that they explicitly do not exist. This is mostly for record keeping when something is known to not be converted but can also be useful when the corresponding names item is NULL.

Value

If checks are successful TRUE invisibly, if not other output depending on the context

Author(s)

Luke Zappia

writeH5AD

Write H5AD

Description

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

Usage

```
writeH5AD(
  sce,
  file,
  X_name = NULL,
  skip_assays = FALSE,
  compression = c("none", "gzip", "lzf"),
  version = NULL,
  verbose = NULL,
  ...
)
```

Arguments

sce	A SingleCellExperiment object.
file	String containing a path to write the new .h5ad file.
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.
skip_assays	Logical scalar indicating whether assay matrices should be ignored when writing to file.
compression	Type of compression when writing the new .h5ad file.
version	A string giving the version of the anndata Python library to use. Allowed values are available in <code>.AnnDataVersions</code> . By default the latest version is used.
verbose	Logical scalar indicating whether to print progress messages. If NULL uses <code>getOption("zellkonverter.verbose")</code> .
...	Arguments passed on to SCE2AnnData <code>assays, colData, rowData, reducedDims, metadata, colPairs, rowPairs</code> Arguments specifying how these slots are converted. If TRUE everything in that slot is converted, if FALSE nothing is converted and if a character vector only those items or columns are converted.

Details**Skipping assays:**

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.

DelayedArray assays:

If `sce` contains any **DelayedArray** matrices as assays `writeH5AD()` will write them to disk using the **rhdf5** package directly rather than via Python to avoid instantiating them in memory. However there is currently an issue which prevents this being done for sparse **DelayedArray** matrices.

Known conversion issues:*Coercion to factors:*

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.

Environment:

See [AnnData-Environment](#) for more details on **zellkonverter** Python environments.

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

AnnData-Environment, 6
.AnnDataVersions (AnnData-Environment),
6

AnnData-Conversion, 3
AnnData-Environment, 6, 10, 13
AnnData2SCE, 9
AnnData2SCE (AnnData-Conversion), 3
AnnData2SCE(), 10
AnnDataDependencies
(AnnData-Environment), 6

basilisk::BasiliskEnvironment(), 6, 7
basilisk::basiliskRun(), 7
basilisk::basiliskStart(), 7
basilisk::setBasiliskShared(), 6

DataFrame, 5
dgCMatrix, 5

expectSCE, 7

int_metadata(), 5

metadata(), 5

py_to_r.numpy.ndarray
(r-py-conversion), 8

r-py-conversion, 8
readH5AD, 9
readH5AD(), 5, 14
reticulate::py_to_r(), 8
rowData(), 5

SCE2AnnData, 13
SCE2AnnData (AnnData-Conversion), 3
SCE2AnnData(), 14
setZellkonverterVerbose, 10
SingleCellExperiment, 3-5, 7, 9-14

validateH5ADSCE, 11

writeH5AD, 12
writeH5AD(), 5, 10

zellkonverter (zellkonverter-package), 2
zellkonverter-package, 2
zellkonverterAnnDataEnv
(AnnData-Environment), 6