Package ‘zellkonverter’

May 11, 2024

Title  Conversion Between scRNA-seq Objects
Version  1.14.0
Date  2024-04-26

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  7.3.1
Language  en-GB
StagedInstall  no
VignetteBuilder  knitr

git_url  https://git.bioconductor.org/packages/zellkonverter
git_branch  RELEASE_3_19
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](https://github.com/theislab/zellkonverter)
- Report bugs at [https://github.com/theislab/zellkonverter/issues](https://github.com/theislab/zellkonverter/issues)

---

**AnnData-Conversion**

*Convert between AnnData and SingleCellExperiment*

**Description**

Conversion between Python AnnData objects and *SingleCellExperiment* objects.

**Usage**

```r
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
)
```

```r
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):
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**

```r
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:
  })
}
```
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 with 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 the 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**

```r
$.AnnDataVersions
AnnDataDependencies()
AnnDataDependencies(version = "0.7.6")

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

**Description**

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

**Usage**

```r
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**

```r
## 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
Description

Reads a H5AD file and returns a SingleCellExperiment object.

Usage

```r
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 .AnnDataVersions. By default the latest version is used.
- **verbose**: Logical scalar indicating whether to print progress messages. If NULL uses getOption("zellkonverter.verbose").
- **...**: Arguments passed on to AnnData2SCE

  - **layers,uns,var,obs,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**

```r
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**

```r
setZellkonverterVerbose(verbos = TRUE)
```

**Arguments**

- **verbose** Logical value for the verbosity option.
validateH5ADSCE

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

sce A SingleCellExperiment object.
names Named list of expected names. Names are slots and values are vectors of names that are expected to exist in that slot.
missing 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**

```r
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 `.AnnDataVersions`. By default the latest version is used.
- **verbose**  
  Logical scalar indicating whether to print progress messages. If `NULL` uses `getOption("zellkonverter.verbose")`.
- **...**  
  Arguments passed on to `SCE2AnnData`.

**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