Package ‘zellkonverter’

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Title Conversion Between scRNA-seq Objects
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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.

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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.

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See Also

Useful links:

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

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Convert AnnData between 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 \texttt{SCE2AnnData()}, matrices are converted to a \texttt{numpy}-friendly format. Sparse matrices are converted to \texttt{dgCMatrix} objects while all other matrices are converted into ordinary matrices. If \texttt{skip\_assays = TRUE}, empty sparse matrices are created instead and the user is expected to fill in the assays on the Python side.

For \texttt{AnnData2SCE()}, a warning is raised if there is no corresponding R format for a matrix in the \texttt{AnnData} object, and an empty sparse matrix is created instead as a placeholder. If \texttt{skip\_assays = NA}, no warning is emitted but variables are created in the \texttt{int\_metadata()} of the output to specify which assays were skipped.

If \texttt{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 \texttt{readH5AD()} for an example.

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

Values stored in the \texttt{varm} slot of an \texttt{AnnData} object are stored in a column of \texttt{rowData()} in a \texttt{SingleCellExperiment} as a DataFrame of matrices. If this column is present an attempt is made to transfer this information when converting from \texttt{SingleCellExperiment} to \texttt{AnnData}.

\textbf{Value}

\texttt{AnnData2SCE()} will return a \texttt{SingleCellExperiment} containing the equivalent data from \texttt{adata}.

\texttt{SCE2AnnData()} will return a \texttt{reticulate} reference to an \texttt{AnnData} object containing the content of \texttt{sce}.

\textbf{Author(s)}

Luke Zappia

Aaron Lun

\textbf{See Also}

\texttt{writeH5AD()} and \texttt{readH5AD()} for dealing directly with H5AD files.

\textbf{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:
  })
}
```
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

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")

c1 <- basilisk::basiliskStart(zellkonverterAnnDataEnv())
anndata <- reticulate::import("anndata")
basilisk::basiliskStop(c1)
```

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
readH5AD

**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 usesgetOption("zellkonverter.verbose").
- **...** 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(verbos = 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

```r
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
writeH5AD

- 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

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 .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

```r
# 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)
}
```
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