

Package ‘BiocSklern’

November 22, 2024

Title interface to python sklearn via Rstudio reticulate

Description This package provides interfaces to selected sklearn elements, and demonstrates fault tolerant use of python modules requiring extensive iteration.

Version 1.29.0

Suggests testthat, HDF5Array, BiocStyle, rmarkdown, knitr

Depends R (>= 4.0), reticulate, methods, SummarizedExperiment

Imports basilisk

License Artistic-2.0

LazyLoad yes

biocViews StatisticalMethod, DimensionReduction, Infrastructure

RoxygenNote 7.3.1

VignetteBuilder knitr

SystemRequirements python (>= 2.7), sklearn, numpy, pandas, h5py

Roxygen list(markdown=TRUE)

Encoding UTF-8

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

git_branch devel

git_last_commit 8c69d92

git_last_commit_date 2024-10-29

Repository Bioconductor 3.21

Date/Publication 2024-11-22

Author Vince Carey [cre, aut]

Maintainer Vince Carey <stvjc@channing.harvard.edu>

Contents

h5mat	2
H5matref	3
SkDecomp	4

SkDecomp-class	4
skIncrPartialPCA	5
skIncrPCA	6
skIncrPCA_h5	6
skIncrPPCA	7
skKMeans	9
skPartialPCA_step	10
skPCA	11
skPWD	11

Index 13

h5mat	<i>create a file connection to HDF5 matrix</i>
-------	--

Description

create a file connection to HDF5 matrix

Usage

```
h5mat(infile, mode = "r", ...)
```

Arguments

infile	a pathname to an HDF5 file
mode	character(1) defaults to "r", see <code>py_help</code> for <code>h5py.File</code>
...	unused

Value

instance of (S3) `h5py._hl.files.File`

Note

The result of this function must be used with `basiliskRun` with the `env` argument set to `bsklenv`, or there is a risk of inconsistent python modules being invoked. This should only be used with the persistent environment discipline of `basilisk`.

Examples

```
if (interactive()) { # not clear why
fn = system.file("ban_6_17/assays.h5", package="BiocSklern")
proc = basilisk::basiliskStart(BiocSklern::bsklenv)
basilisk::basiliskRun(proc, function(infile, mode="r") {
  h5py = reticulate::import("h5py")
  hh = h5py$File( infile, mode=mode )
  cat("File reference:\n ")
  print(hh)
})
}
```

```
cat("File attributes in python:\n ")
print(head(names(hh)))
cat("File keys in python:\n ")
print(hh$keys())
cat("HDF5 dataset in python:\n ")
print(hh['assay001'])
}, infile=fn, mode="r")
basilisk::basiliskStop(proc)
}
```

H5matref

obtain an HDF5 dataset reference suitable for handling as numpy matrix

Description

obtain an HDF5 dataset reference suitable for handling as numpy matrix

Usage

```
H5matref(filename, dsname = "assay001")
```

Arguments

filename	a pathname to an HDF5 file
dsname	internal name of HDF5 matrix to use, defaults to 'assay001'

Value

instance of (S3) "h5py._hl.dataset.Dataset"

Note

This should only be used with persistent environment discipline of basilisk. Additional support is planned in Bioc 3.12.

Examples

```
fn = system.file("ban_6_17/assays.h5", package="BiocSklern")
ban = H5matref(fn)
ban
proc = basilisk::basiliskStart(BiocSklern::bsklenv)
fullpca = basilisk::basiliskRun(proc, function() {
  np = import("numpy", convert=FALSE) # ensure
  print(ban$shape)
  print(np$take(ban, 0:3, 0L))
  fullpca = skPCA(ban)
  tx = getTransformed(fullpca)
  print(dim(tx))
})
```

```

    fullpca
  })
  basilisk::basiliskStop(proc)
  # project samples
  np = reticulate::import("numpy", convert=FALSE, delay_load=TRUE)
  np$take(ban, 0:20, 0L)$shape
  st = skPartialPCA_step(np$take(ban, 0:20, 0L), n_comp=4L)
  st = skPartialPCA_step(np$take(ban, 21:40, 0L), n_comp=4L, obj=st)
  st = skPartialPCA_step(np$take(ban, 41:63, 0L), n_comp=4L, obj=st)
  oo = st$transform(ban)
  dim(oo)
  cor(oo[,1:4], getTransformed(fullpca)[,1:4])

```

SkDecomp	<i>constructor for SkDecomp</i>
----------	---------------------------------

Description

constructor for SkDecomp

Usage

SkDecomp(transform, method)

Arguments

transform	typically a numerical matrix representing a projection of the input
method	character(1) arbitrary tag describing the decomposition

SkDecomp-class	<i>container for sklearn objects and transforms</i>
----------------	---

Description

container for sklearn objects and transforms

Usage

```

## S4 method for signature 'SkDecomp'
getTransformed(x)

```

Arguments

x	instance of SkDecomp
---	----------------------

Value

the getTransformed method returns a matrix

Slots

transform stored as R matrix

method string identifying method

Note

In Bioc 3.11, the object slot is removed. This is a consequence of adoption of basilisk discipline for acquiring and using python resources, which greatly increases reliability, at the expense of added complication in handling python objects interactively in R. We are working on restoring this functionality but it will take time.

skIncrPartialPCA	<i>use basilisk discipline to perform partial (n_components) incremental (chunk.size) PCA with scikit.decomposition</i>
------------------	---

Description

use basilisk discipline to perform partial (n_components) incremental (chunk.size) PCA with scikit.decomposition

Usage

```
skIncrPartialPCA(mat, n_components, chunk.size = 10)
```

Arguments

mat a matrix

n_components integer(1) number of PCs to compute

chunk.size integer(1) number of rows to use each step

Note

A good source for capabilities and examples is at the [sklearn doc site](#).

Examples

```
lk = skIncrPartialPCA(iris[,1:4], n_components=3L)
lk
head(getTransformed(lk))
```

skIncrPCA *use sklearn IncrementalPCA procedure*

Description

use sklearn IncrementalPCA procedure

Usage

```
skIncrPCA(mat, n_components = 2L, batch_size = 5L, ...)
```

Arguments

mat	a matrix – can be R matrix or numpy.ndarray, if the latter it must be set up in a basilisk persistent environment, and that is not currently demonstrated for this package.
n_components	number of PCA to retrieve
batch_size	number of records to use at each iteration
...	passed to python IncrementalPCA

Value

matrix with rotation

Examples

```
dem = skIncrPCA(iris[,1:4], batch_size=25L)
dem2 = skIncrPCA(iris[,1:4], batch_size=25L, n_components=2L)
dem
dem2
```

skIncrPCA_h5 *demo of HDF5 processing with incremental PCA/batch_size/fit_transform*

Description

demo of HDF5 processing with incremental PCA/batch_size/fit_transform

Usage

```
skIncrPCA_h5(fn, dsname = "assay001", n_components, chunk.size = 10L)
```

Arguments

fn	character(1) path to HDF5 file
dsname	character(1) name of dataset within HDF5 file, assumed to be 2-dimensional array
n_components	numeric(1) passed to IncrementalPCA
chunk.size	numeric(1) passed to IncrementalPCA as batch_size

Note

Here we use `IncrementalPCA$fit_transform` and let python take care of chunk retrieval. `skIncrPartialPCA` acquires chunks from R matrix and uses `IncrementalPCA$partial_fit`.

Examples

```
if (interactive()) {  
  fn = system.file("hdf5/irmatt.h5", package="BiocSklern") # 'transposed' relative to R iris  
  dem = skIncrPCA_h5(fn, n_components=3L, dsname="tquants")  
  dem  
  head(getTransformed(dem))  
}
```

skIncrPPCA	<i>optionally fault tolerant incremental partial PCA for projection of samples from SummarizedExperiment</i>
------------	--

Description

optionally fault tolerant incremental partial PCA for projection of samples from SummarizedExperiment

Usage

```
skIncrPPCA(  
  se,  
  chunksize,  
  n_components,  
  assayind = 1,  
  picklePath = "./skIdump.pkl",  
  matTx = force,  
  ...  
)
```

Arguments

se	instance of SummarizedExperiment
chunksize	integer number of samples per step
n_components	integer number of PCs to compute
assayind	not used, assumed set to 1
picklePath	if non-null, incremental results saved here via joblib.dump, for each chunk. If NULL, no saving of incremental results.
matTx	a function defaulting to force() that accepts a matrix and returns a matrix with identical dimensions, e.g., function(x) log(x+1)
...	not used

Value

python instance of sklearn.decomposition.incremental_pca.IncrementalPCA

Note

Will treat samples as records and all features (rows) as attributes, projecting. to an n_components-dimensional space. Method will acquire chunk of assay data and transpose before computing PCA contributions. In case of crash, restore from picklePath using joblib\$load after loading reticulate. You can use the n_samples_seen_ component of the restored python reference to determine where to restart. You can manage resumption using skPartialPCA_step.

Examples

```
# demo SE made with TENxGenomics:
# mm = matrixSummarizedExperiment(h5path, 1:27998, 1:750)
# saveHDF5SummarizedExperiment(mm, "tenx_750")
#
if (FALSE) {
if (requireNamespace("HDF5Array")) {
se750 = HDF5Array::loadHDF5SummarizedExperiment(
system.file("hdf5/tenx_750", package="BiocSklern"))
lit = skIncrPPCA(se750[, 1:50], chunksize=5, n_components=4)
round(cor(pypc <- lit$transform(dat <- t(as.matrix(assay(se750[,1:50]))))),3)
rpc = prcomp(dat)
round(cor(rpc$x[,1:4], pypc), 3)
} # this has to be made basilisk-compliant
} # and is blocked until then
```

skKMeans	<i>interface to sklearn.cluster.KMeans using basilisk discipline</i>
----------	--

Description

interface to sklearn.cluster.KMeans using basilisk discipline

Usage

```
skKMeans(mat, ...)
```

Arguments

mat	a matrix-like datum or reference to such
...	arguments to sklearn.cluster.KMeans

Value

a list with cluster assignments (integers starting with zero) and asserted cluster centers.

Note

This is a demonstrative interface to the resources of sklearn.cluster. In this particular interface, we are using sklearn.cluster.k_means_.KMeans. There are many other possibilities in sklearn.cluster: *_dbscan_inner*, *feature_agglomeration*, *hierarchical*, *k_means*, *k_means_elkan*, *affinity_propagation*, *bicluster*, *birch*, *dbscan*, *hierarchical*, *k_means*, *mean_shift*, *setup*, *spectral*.

Basilisk discipline has not been used for this function, 1 June 2022.

Examples

```
irloc = system.file("csv/iris.csv", package="BiocSklern")
np = reticulate::import("numpy", delay_load=TRUE, convert=FALSE)
h5py = reticulate::import("h5py", delay_load=TRUE)
irismat = np$genfromtxt(irloc, delimiter=',')
ans = skKMeans(irismat, n_clusters=2L)
names(ans) # names of available result components
table(iris$Species, ans$labels)
# now use an HDF5 reference
irh5 = system.file("hdf5/irmat.h5", package="BiocSklern")
fref = h5py$File(irh5)
ds = fref$`__getitem__`("quants")
ans2 = skKMeans(np$array(ds)$T, n_clusters=2L) # HDF5 matrix is transposed relative to python array layout! Is the
table(ans$labels, ans2$labels)
ans3 = skKMeans(np$array(ds)$T,
  n_clusters=8L, max_iter=200L,
  algorithm="lloyd", random_state=20L)
dem = skKMeans(iris[,1:4], n_clusters=3L, max_iter=100L, algorithm="lloyd",
  random_state=20L)
```

```

str(dem)
tab = table(iris$Species, dem$labels)
tab
plot(iris[,1], iris[,3], col=as.numeric(factor(iris$Species)))
points(dem$centers[,1], dem$centers[,3], pch=19, col=apply(tab,2,which.max))

```

skPartialPCA_step *take a step in sklearn IncrementalPCA partial fit procedure*

Description

take a step in sklearn IncrementalPCA partial fit procedure

Usage

```
skPartialPCA_step(mat, n_components, obj)
```

Arguments

mat	a matrix – can be R matrix or numpy.ndarray
n_components	number of PCA to retrieve
obj	sklearn.decomposition.IncrementalPCA instance

Value

trained IncrementalPCA reference, to which 'transform' method can be applied to obtain projection for any compliant input

Note

if obj is missing, the process is initialized with the matrix provided

Examples

```

# these steps are not basilisk-compliant, you need to acquire references
irloc = system.file("csv/iris.csv", package="BiocSklern")
np = reticulate::import("numpy", delay_load=TRUE, convert=FALSE)
irismat = np$genfromtxt(irloc, delimiter=',')
ta = np$take
ipc = skPartialPCA_step(ta(irismat,0:49,0L))
ipc = skPartialPCA_step(ta(irismat,50:99,0L), obj=ipc)
ipc = skPartialPCA_step(ta(irismat,100:149,0L), obj=ipc)
head(names(ipc))
ipc$transform(ta(irismat,0:5,0L))
fullproj = ipc$transform(irismat)
fullpc = prcomp(data.matrix(iris[,1:4]))$x
round(cor(fullpc,fullproj),3)

```

skPCA	<i>use sklearn PCA procedure</i>
-------	----------------------------------

Description

use sklearn PCA procedure

Usage

```
skPCA(mat, ...)
```

Arguments

mat	a matrix – can be R matrix or numpy.ndarray
...	additional parameters passed to sklearn.decomposition.PCA, for additional information use <code>py_help()</code> on a reticulate-imported <code>sklearn.decomposition.PCA</code> instance.

Value

matrix with rotation

Note

If no additional arguments are passed, all defaults are used.

Examples

```
#irloc = system.file("csv/iris.csv", package="BiocSklern")
#irismat = SklearnEls()$np$genfromtxt(irloc, delimiter=',')
#skpi = skPCA(irismat)
#getTransformed(skpi)[1:5,]
chk = skPCA(data.matrix(iris[,1:4]))
chk
head(getTransformed(chk))
head(prcomp(data.matrix(iris[,1:4]))$x)
```

skPWD	<i>use sklearn pairwise_distances procedure</i>
-------	---

Description

use sklearn pairwise_distances procedure

Usage

```
skPWD(mat, ...)
```

Arguments

`mat` a matrix – can be R matrix or `numpy.ndarray`
`...` additional parameters passed to `sklearn.metrics.pairwise_distances`, for additional information use `py_help()` on a reticulate-imported `sklearn.metrics.pairwise_distances` instance.

Value

matrix with rotation

Note

If no additional arguments are passed, all defaults are used.

Examples

```
irloc = system.file("csv/iris.csv", package="BiocSklern")
data(iris)
irismat = as.matrix(iris[,1:4])
chk1 = skPWD(irismat)
chk1[1:4,1:5]
chk2 = skPWD(irismat, metric='manhattan')
chk2[1:4,1:5]
```

Index

[getTransformed \(SkDecomp-class\)](#), [4](#)
[getTransformed, SkDecomp-method](#)
 ([SkDecomp-class](#)), [4](#)

[h5mat](#), [2](#)
[H5matref](#), [3](#)

[SkDecomp](#), [4](#)
[SkDecomp-class](#), [4](#)
[skIncrPartialPCA](#), [5](#)
[skIncrPCA](#), [6](#)
[skIncrPCA_h5](#), [6](#)
[skIncrPPCA](#), [7](#)
[skIncrPPCA, SummarizedExperiment-method](#)
 ([skIncrPPCA](#)), [7](#)

[skKMeans](#), [9](#)
[skPartialPCA_step](#), [10](#)
[skPCA](#), [11](#)
[skPWD](#), [11](#)