

# Package ‘BiocSklern’

December 23, 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** 1.28.0

**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

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h5mat	<i>create a file connection to HDF5 matrix</i>
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## 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 py_help for h5py.File
...	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)
}
```

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H5matref	<i>obtain an HDF5 dataset reference suitable for handling as numpy matrix</i>
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---

### 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])
```

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SkDecomp	<i>constructor for SkDecomp</i>
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**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

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

**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.

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

**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	<i>use sklearn IncrementalPCA procedure</i>
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---

**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
```

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skIncrPCA_h5	<i>demo of HDF5 processing with incremental PCA/batch_size/fit_transform</i>
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---

**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>
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---

## 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

*interface to sklearn.cluster.KMeans using basilisk discipline***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
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(iris.mat,100:149,0L), obj=ipc)
head(names(ipc))
ipc$transform(ta(iris.mat,0:5,0L))
fullproj = ipc$transform(iris.mat)
fullpc = prcomp(data.matrix(iris[,1:4]))$x
round(cor(fullpc,fullproj),3)
```

---

skPCA

*use sklearn PCA procedure*


---

### 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 `py_help()` on a reticulate-imported `sklearn.decomposition.PCA` instance.

### Value

matrix with rotation

### Note

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

### Examples

```
#irloc = system.file("csv/iris.csv", package="BiocSklearn")
#iris.mat = SklearnEls()$np$genfromtxt(irloc, delimiter=',')
#skpi = skPCA(iris.mat)
#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]
```

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