

Package ‘SCArray.sat’

May 11, 2024

Type Package

Title Large-scale single-cell RNA-seq data analysis using GDS files and Seurat

Version 1.4.0

Date 2024-04-24

Depends methods, SCArray (>= 1.7.13), SeuratObject (>= 5.0), Seurat (>= 5.0)

Imports S4Vectors, utils, stats, BiocGenerics, BiocParallel, gdsfmt, DelayedArray, BiocSingular, SummarizedExperiment, Matrix

Suggests future, RUnit, knitr, markdown, rmarkdown, BiocStyle

Description Extends the Seurat classes and functions to support Genomic Data Structure (GDS) files as a DelayedArray backend for data representation. It relies on the implementation of GDS-based DelayedMatrix in the SCArray package to represent single cell RNA-seq data. The common optimized algorithms leveraging GDS-based and single cell-specific DelayedMatrix (SC_GDSMatrix) are implemented in the SCArray package. SCArray.sat introduces a new SCArrayAssay class (derived from the Seurat Assay), which wraps raw counts, normalized expressions and scaled data matrix based on GDS-specific DelayedMatrix. It is designed to integrate seamlessly with the Seurat package to provide common data analysis in the SeuratObject-based workflow. Compared with Seurat, SCArray.sat significantly reduces the memory usage without downsampling and can be applied to very large datasets.

License GPL-3

VignetteBuilder knitr

BugReports <https://github.com/AbbVie-ComputationalGenomics/SCArray/issues>

biocViews DataRepresentation, DataImport, SingleCell, RNASeq

git_url <https://git.bioconductor.org/packages/SCArray.sat>

git_branch RELEASE_3_19

git_last_commit 57e551e

git_last_commit_date 2024-04-30

Repository Bioconductor 3.19

Date/Publication 2024-05-10

Author Xiuwen Zheng [aut, cre] (<<https://orcid.org/0000-0002-1390-0708>>),
Seurat contributors [ctb] (for the classes and methods defined in
Seurat)

Maintainer Xiuwen Zheng <xiuwen.zheng@abbvie.com>

Contents

SCArray.sat-package	2
CreateAssayObject2	3
NormalizeData	4
RunPCA	5
ScaleData	7
SCArrayAssay-class	9
SCArrayAssay-methods	9
scGetFiles	10
scMemory	11
scNewAssayGDS	12
scNewSeuratGDS	13
Seurat_g-class	14

Index **15**

SCArray.sat-package *Large-scale single-cell RNA-seq data analysis using GDS files and Seurat*

Description

The package extends the Seurat classes and functions to support GDS files as a DelayedArray backend for data representation. It introduces a new SCArrayAssay class (derived from the Seurat Assay), which wraps raw counts, normalized expressions and scaled data matrix based on DelayedMatrix. It is designed to integrate seamlessly with the SeuratObject and Seurat packages to provide common data analysis, with the optimized algorithms for GDS data files.

Details

Package: SCArray.sat
Type: Package
License: GPL version 3

Author(s)

Xiuwen Zheng

`CreateAssayObject2` *Create an Assay object*

Description

Create an `SCArrayAssay` (inherited from `Assay`) object from counts or prenormalized data.

Usage

```
CreateAssayObject2(counts, data, min.cells=0, min.features=0,  
  key=NULL, check.matrix=FALSE, ...)
```

Arguments

<code>counts</code>	Unnormalized raw counts (matrix, <code>dgCMatrx</code> or <code>DelayedMatrix</code>)
<code>data</code>	Prenormalized data (matrix, <code>dgCMatrx</code> or <code>DelayedMatrix</code>)
<code>min.cells</code>	if > 0, a lower cutoff for filtering cells
<code>min.features</code>	if > 0, a lower cutoff for filtering features
<code>check.matrix</code>	Check counts matrix for NA, NaN, Inf, and non-integer values
<code>key</code>	Key name for the assay
<code>...</code>	Arguments passed to <code>as.sparse</code> when counts or data is matrix or <code>dgCMatrx</code>

Details

Similar to `SeuratObject::CreateAssayObject()`, except allowing `DelayedMatrix` counts or data, and returning a `SCArrayAssay` object. counts and data should not be provided at the same time.

Value

Return an instance of `SCArrayAssay`.

Author(s)

Xiuwen Zheng

See Also

[CreateAssayObject](#), [scGetFiles](#)

Examples

```
fn <- system.file("extdata", "example.gds", package="SCArray")

x <- scArray(fn, "counts")
colnames(x) <- paste0("c", 1:ncol(x))
rownames(x) <- paste0("g", 1:nrow(x))
x

a <- CreateAssayObject2(x)
a

scGetFiles(x)
scGetFiles(a)

remove(x, a)
```

 NormalizeData

Normalize Count Data

Description

Normalizes the count data in the Seurat assay.

Usage

```
# NormalizeData(object, ...)
## S3 method for class 'SC_GDSMatrix'
NormalizeData(object,
  normalization.method="LogNormalize", scale.factor=1e4, margin=1,
  verbose=TRUE, ...)
```

Arguments

object	input R object (e.g., a SC_GDSMatrix object)
normalization.method	"LogNormalize", "CLR" or "RC"; see <code>NormalizeData.Seurat</code> for more details
scale.factor	the scale factor for cell-level normalization
margin	only applicable when <code>normalization.method="CLR"</code> , normalize across features (<code>margin=1</code>) or cells (<code>margin=2</code>)
verbose	if TRUE, show information
...	additional arguments passed to specific methods

Details

`NormalizeData()` does not store the normalized data in a GDS file, since the calculation is "delayed" until it is needed.

Value

Returns a SC_GDSMatrix matrix.

Author(s)

Xiuwen Zheng

See Also

[NormalizeData](#)

Examples

```
fn <- system.file("extdata", "example.gds", package="SCArray")

d <- scNewSeuratGDS(fn)
d
d <- NormalizeData(d)

remove(a, d)
```

RunPCA

Run PCA

Description

Performs PCA on a Seurat SCArrayAssay or a DelayedMatrix object.

Usage

```
# RunPCA(object, ...)
## S3 method for class 'SCArrayAssay'
RunPCA(object, assay=NULL, features=NULL, npcs=50,
        rev.pca=FALSE, weight.by.var=TRUE, verbose=TRUE, ndims.print=1:5,
        nfeatures.print=30, reduction.key="PC_", seed.use=42, ...)
## S3 method for class 'SC_GDSMatrix'
RunPCA(object, assay=NULL, npcs=50, rev.pca=FALSE,
        weight.by.var=TRUE, verbose=TRUE, ndims.print=1:5,
        nfeatures.print=30, reduction.key="PC_", seed.use=42, approx=TRUE,
        BPPARAM, ...)
```

Arguments

object	input R object (e.g., a SCArrayAssay object)
assay	NULL for using the active assay, or an assay name
features	if NULL, PCA will be run on the scaled data; otherwise, features to compute PCA on

<code>npcs</code>	# of top PCs to be calculated
<code>rev.pca</code>	By default (FALSE), perform PCA on the cell x gene matrix; otherwise, compute it on gene x cell matrix
<code>weight.by.var</code>	if TRUE, weight the cell embeddings (when <code>rev.pca=FALSE</code>) or the the gene loadings (when <code>rev.pca=TRUE</code>) by the variance of each PC
<code>verbose</code>	if TRUE, show information
<code>ndims.print</code>	which PCs to print genes for
<code>nfeatures.print</code>	# of genes to print for each PC
<code>reduction.key</code>	dimensional reduction key
<code>seed.use</code>	a random seed; or NULL for not setting a seed internally
<code>approx</code>	if TRUE, use <code>IrlbaSVD</code> ; otherwise use <code>ExactSVD</code>
<code>BPPARAM</code>	NULL for non-parallel execution, or a <code>BiocParallelParam</code> object for parallelization; if it is missing, <code>getAutoBPPARAM()</code> will be used
<code>...</code>	additional arguments passed to specific methods

Details

`RunPCA()` computes the covariance matrix of genes (if # of genes \leq # of cells) or the cell covariance matrix for the PCA calculation, which can reduce the times of accessing on-disk data.

Value

Return a data frame for reduction data (via `CreateDimReducObject`).

Author(s)

Xiuwen Zheng

See Also

[RunPCA](#), [CreateDimReducObject](#), [BiocParallelParam](#), [getAutoBPPARAM](#)

Examples

```
fn <- system.file("extdata", "example.gds", package="SCArray")

d <- scNewSeuratGDS(fn)

d <- NormalizeData(d)
d <- FindVariableFeatures(d, nfeatures=250)
d <- ScaleData(d)

d <- RunPCA(d, ndims.print=1:2)
DimPlot(d, reduction="pca")

remove(a, d)
```

Description

Scales and centers features or residuals in the dataset.

Usage

```
# ScaleData(object, ...)
## S3 method for class 'SC_GDSMatrix'
ScaleData(object, features=NULL, vars.to.regress=NULL,
  latent.data=NULL, split.by=NULL, model.use='linear', use.umi=FALSE,
  do.scale=TRUE, do.center=TRUE, scale.max=10, block.size=1000,
  min.cells.to.block=3000, verbose=TRUE, use_gds=TRUE, rm_tmpfile=TRUE, ...)
```

Arguments

object	input R object (e.g., a SC_GDSMatrix object)
features	if NULL, to use the variable features (found via FindVariableFeatures()); or features names to scale/center
vars.to.regress	NULL or variable names to regress out
latent.data	NULL or a data.frame to regress out the covariates
split.by	variable name in the metadata, or a vector or factor defining grouping of cells
model.use	regression model: "linear" (default), "poisson" or "negbinom"
use.umi	only applicable when the covariates are given in vars.to.regress for regression; default is FALSE for linear regression, TRUE for negbinom and poisson models
do.scale	if TRUE, scale the data
do.center	if TRUE, center the data
scale.max	max value in the resulting scaled data; see ScaleData.Seurat for more details
block.size	not used
min.cells.to.block	not used
verbose	if TRUE, show information
use_gds	if TRUE, use SC_GDSMatrix for the scaled data; if FALSE, to use a dense in-memory scaled matrix; or a GDS file name for storing the resulting data matrix; see details
rm_tmpfile	if TRUE, remove any temporary GDS file after the calculation; the temporary file will be created when calculating the residuals
...	additional arguments passed to specific methods

Details

ScaleData() stores the scaled data in a GDS file when use_gds=TRUE or an output GDS file name is given via use_gds. When vars.to.regress and split.by are both NULL, an output GDS file is not needed, since the resulting DelayedMatrix can be represented as common operations on the count matrix. If use_gds=TRUE, an output file name "_scale_data.gds" will be used if it does not exist, or "_scale_data2.gds" (if not exists), "_scale_data3.gds" and so on. If use_gds is an output file name, the resulting data matrix will be saved to a GDS file. When vars.to.regress are given, a temporary GDS file (e.g., "_temp_scale_data.gds", use_gds with a prefix "_temp") will be created to store the residuals before scaling. This temporary file will be deleted after the calculation when rm_tmpfile=TRUE.

Value

Returns a SC_GDSMatrix matrix if use_gds=TRUE or use_gds is an output file name, otherwise returns an in-memory matrix.

Author(s)

Xiuwen Zheng

See Also

[ScaleData](#)

Examples

```
fn <- system.file("extdata", "example.gds", package="SCArray")

d <- scNewSeuratGDS(fn)

d <- NormalizeData(d)
d <- FindVariableFeatures(d, nfeatures=50)
d <- ScaleData(d)

GetAssayData(d, slot="scale.data") # DelayedMatrix

# scale with split.by
ss <- rep(c(TRUE, FALSE), length.out=ncol(d))
d <- ScaleData(d, split.by=ss)

fn <- scGetFiles(d)
fn[2L] # the file name storing scaled data

remove(a, d)
unlink(fn[grep("^_scale", fn)], force=TRUE)
```

SCArrayAssay-class *GDS-specific Assay Class*

Description

The SCArrayAssay class extends the Assay class of Seurat with the new slots counts2, data2 and scale.data2 replacing counts, data and scale.data.

Slots

counts2 Unnormalized raw counts (dgCMatrx or SC_GDSMatrix), replacing Assay@counts

data2 Normalized expression data (dgCMatrx or SC_GDSMatrix), replacing Assay@data

scale.data2 Scaled expression data (NULL, matrix or SC_GDSMatrix), replacing Assay@scale.data

Author(s)

Xiuwen Zheng

See Also

[Assay-class](#), [Seurat_g-class](#), [GetAssayData](#), [SetAssayData](#)

SCArrayAssay-methods *SCArrayAssay S3 methods*

Description

Gets and sets data in the Seurat Assay object.

Usage

```
## S3 method for class 'SCArrayAssay'
GetAssayData(object,
  slot=c("data", "scale.data", "counts"), ...)
## S3 method for class 'SCArrayAssay'
SetAssayData(object, layer, new.data,
  slot=c('data', 'scale.data', 'counts'), ...)

## S3 method for class 'SCArrayAssay'
subset(x, cells=NULL, features=NULL, ...)
```

Arguments

object, x	a SCArrayAssay object (inherited from SeuratObject::Assay)
layer	layer
new.data	a new data matrix (dgCMatrx or SC_GDSMatrix)
slot	data matrix in the Assay object, "data" is used by default
cells	names or indices for selected cells
features	names or indices for selected features
...	further arguments to be passed to or from other methods

Value

Return a data matrix or an instance of [SCArrayAssay](#).

Author(s)

Xiuwen Zheng

See Also

[Assay](#)

scGetFiles

File names for on-disk backend

Description

Get a list of file names for DelayedArray with an on-disk backend.

Usage

```
scGetFiles(object, ...)
## S4 method for signature 'Assay'
scGetFiles(object, ...)
## S4 method for signature 'SCArrayAssay'
scGetFiles(object, ...)
## S4 method for signature 'Seurat'
scGetFiles(object, ...)
```

Arguments

object	input R object (e.g., a Seurat object)
...	additional arguments passed to specific methods

Value

Return a character vector storing file names.

Author(s)

Xiuwen Zheng

See Also[scGetFiles](#)**Examples**

```
fn <- system.file("extdata", "example.gds", package="SCArray")

a <- scNewAssayGDS(fn)
d <- Seurat::CreateSeuratObject(a)

scGetFiles(a)
scGetFiles(d)

remove(a, d)
```

scMemory

Load Data to Memory

Description

Loads the internal data to memory for any on-disk object.

Usage

```
scMemory(x, ...)
## S4 method for signature 'SCArrayAssay'
scMemory(x, slot=NULL, ...)
## S4 method for signature 'Seurat'
scMemory(x, assay=NULL, slot=NULL, ...)
```

Arguments

x	input R object (e.g., a Seurat object)
assay	NULL for using the active assay, or a list of assay names
slot	NULL for all "counts", "data" and "scale.data"; or a character vector including "counts", "data" or "scale.data"; see details
...	additional arguments passed to specific methods

Details

If slot=NULL, return a Assay object instead of SCArrayAssay object, so it can downgrade a SCArrayAssay object to a Assay object.

Value

Return an object (it maybe a different type from `class(x)`).

Author(s)

Xiuwen Zheng

See Also

[scMemory](#)

Examples

```
fn <- system.file("extdata", "example.gds", package="SCArray")

d1 <- scNewSeuratGDS(fn)
is(GetAssay(d1))

d2 <- scMemory(d1)
is(GetAssay(d2))

remove(a, d1, d2)
```

scNewAssayGDS

Create Assay Object

Description

Creates a new Seurat Assay object (`SCArrayAssay`) from a GDS file.

Usage

```
scNewAssayGDS(gdsfile, name="counts", key="rna_", row_data=TRUE, check=TRUE,
  verbose=TRUE)
```

Arguments

<code>gdsfile</code>	a file name for the GDS file, or a <code>SCArrayFileClass</code> object
<code>name</code>	characters for the name of data matrix in the GDS file; if <code>NA_character_</code> , to use the first assay
<code>key</code>	characters for the Assay key
<code>row_data</code>	if <code>TRUE</code> , add <code>rowData()</code> to the feature-level meta data of the Seurat Assay
<code>check</code>	if <code>TRUE</code> , check the feature names
<code>verbose</code>	if <code>TRUE</code> , show information

Value

Return an instance of [SCArrayAssay](#).

Author(s)

Xiuwen Zheng

See Also

[SCArrayAssay](#), [SCArrayFileClass](#), [scExperiment](#), [scNewSeuratGDS](#)

Examples

```
# raw count data in a GDS file
fn <- system.file("extdata", "example.gds", package="SCArray")

a <- scNewAssayGDS(fn)
a
class(a)

d <- Seurat::CreateSeuratObject(a)
d

rm(a, d)
```

scNewSeuratGDS	<i>Create Seurat Object</i>
----------------	-----------------------------

Description

Creates a new Seurat object from a GDS file.

Usage

```
scNewSeuratGDS(gdsfile, assay.name=NULL, key=c(counts="rna_"), row_data=TRUE,
  col_data=TRUE, check=TRUE, verbose=TRUE)
```

Arguments

gdsfile	a file name for the GDS file, or a SCArrayFileClass object
assay.name	characters for the name of data matrix in the GDS file; if NULL, to use all of the assays
key	a character vector for an assay key map, where its names are the GDS node names
row_data	if TRUE, add <code>rowData()</code> to the feature-level meta data of the first Seurat Assay
col_data	if TRUE, add <code>colData()</code> to the cell-level meta data of the Seurat object
check	if TRUE, check the feature names
verbose	if TRUE, show information

Details

"counts" must be in the input GDS file and it is used as the raw count data in the active Seurat assay. If "logcounts" exists, it is used as normalized data associated with "counts". If there are other data matrices in the GDS file, they will be added to the assay list.

Value

Return an instance of [Seurat](#).

Author(s)

Xiuwen Zheng

See Also

[SCArrayAssay](#), [SCArrayFileClass](#), [scExperiment](#), [scNewAssayGDS](#)

Examples

```
# raw count data in a GDS file
fn <- system.file("extdata", "example.gds", package="SCArray")

d <- scNewSeuratGDS(fn)
d
class(d)

rm(d)
```

Seurat_g-class

GDS-based Seurat Class

Description

The Seurat_g class inherits directly from "Seurat".

Slots

```
setClass("Seurat_g", contains="Seurat")
```

Author(s)

Xiuwen Zheng

See Also

[SCArrayAssay-class](#)

Index

* GDS

- CreateAssayObject2, 3
- NormalizeData, 4
- RunPCA, 5
- ScaleData, 7
- SCArray.sat-package, 2
- SCArrayAssay-class, 9
- SCArrayAssay-methods, 9
- scGetFiles, 10
- scMemory, 11
- scNewAssayGDS, 12
- scNewSeuratGDS, 13
- Seurat_g-class, 14

* SingleCell

- CreateAssayObject2, 3
- SCArray.sat-package, 2
- SCArrayAssay-class, 9
- SCArrayAssay-methods, 9
- scNewAssayGDS, 12
- scNewSeuratGDS, 13
- Seurat_g-class, 14

* methods

- NormalizeData, 4
- RunPCA, 5
- ScaleData, 7
- scGetFiles, 10
- scMemory, 11

as.sparse, 3

Assay, 10

BiocParallelParam, 6

CreateAssayObject, 3

CreateAssayObject2, 3

CreateDimReducObject, 6

GetAssayData, 9

GetAssayData (SCArrayAssay-methods), 9

getAutoBPPARAM, 6

NormalizeData, 4, 5

RunPCA, 5, 6

ScaleData, 7, 8

SCArray.sat (SCArray.sat-package), 2

SCArray.sat-package, 2

SCArrayAssay, 3, 10, 13, 14

SCArrayAssay (SCArrayAssay-class), 9

SCArrayAssay-class, 9

SCArrayAssay-methods, 9

SCArrayFileClass, 13, 14

scExperiment, 13, 14

scGetFiles, 3, 10, 11

scGetFiles, Assay-method (scGetFiles), 10

scGetFiles, SCArrayAssay-method
(scGetFiles), 10

scGetFiles, Seurat-method (scGetFiles),
10

scMemory, 11, 12

scMemory, SCArrayAssay-method
(scMemory), 11

scMemory, Seurat-method (scMemory), 11

scMemory, Seurat_g-method (scMemory), 11

scNewAssayGDS, 12, 14

scNewSeuratGDS, 13, 13

SetAssayData, 9

SetAssayData (SCArrayAssay-methods), 9

Seurat, 14

Seurat_g (Seurat_g-class), 14

Seurat_g-class, 14

subset (SCArrayAssay-methods), 9