Package 'SummarizedExperiment'

March 7, 2018

Description The SummarizedExperiment container contains one or more assays, each represented by a matrix-like object of numeric or other mode. The rows typically represent genomic ranges of interest and the columns represent samples.
Version 1.8.1
Encoding UTF-8
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Maintainer Bioconductor Package Maintainer <maintainer@bioconductor.org< td=""></maintainer@bioconductor.org<>
biocViews Genetics, Infrastructure, Sequencing, Annotation, Coverage, GenomeAnnotation
Depends R (>= 3.2), methods, GenomicRanges (>= 1.29.14), Biobase, DelayedArray (>= 0.3.20)
Imports utils, stats, tools, Matrix, BiocGenerics (>= 0.15.3), S4Vectors (>= 0.13.13), IRanges (>= 2.11.17), GenomeInfoDb (>= 1.13.1)
Suggests annotate, AnnotationDbi, hgu95av2.db, GenomicFeatures, TxDb.Hsapiens.UCSC.hg19.knownGene, BiocStyle, knitr, rmarkdown, digest, jsonlite, rhdf5, HDF5Array (>= 1.5.8), airway, RUnit
VignetteBuilder knitr
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Collate Assays-class.R SummarizedExperiment-class.R RangedSummarizedExperiment-class.R intra-range-methods.R inter-range-methods.R coverage-methods.R findOverlaps-methods.R nearest-methods.R makeSummarizedExperimentFromExpressionSet.R makeSummarizedExperimentFromDataFrame.R readKallisto.R saveHDF5SummarizedExperiment.R zzz.R
NeedsCompilation no

Title SummarizedExperiment container

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Description

The Assays virtual class and its methods provide a formal abstraction of the assays slot of SummarizedExperiment objects.

SimpleListAssays and ShallowSimpleListAssays are concrete subclasses of Assays with the latter being currently the default implementation of Assays objects. Other implementations (e.g. diskbased) could easily be added.

Note that these classes are not meant to be used directly by the end-user and the material in this man page is aimed at package developers.

Details

Assays objects have a list-like semantics with elements having matrix- or array-like semantics (e.g., dim, dimnames).

The Assays API consists of:

- (a) The Assays() constructor function.
- (b) Lossless back and forth coercion from/to SimpleList. The coercion method from SimpleList doesn't need (and should not) validate the returned object.
- (c) length, names, `names<-`, [[, `[[<-`, dim, [, `[<-`, rbind, cbind.

An Assays concrete subclass needs to implement (b) (required) plus, optionally any of the methods in (c).

IMPORTANT: Methods that return a modified Assays object (a.k.a. endomorphisms), that is, [as well as replacement methods names<-, [[<-, and [<-, must respect the *copy-on-change contract*. With objects that don't make use of references internally, the developer doesn't need to take any special action for that because it's automatically taken care of by R itself. However, for objects that do make use of references internally (e.g. environments, external pointers, pointer to a file on disk, etc...), the developer needs to be careful to implement endomorphisms with copy-on-change semantics. This can easily be achieved (and is what the default methods for Assays objects do) by performang a full (deep) copy of the object before modifying it instead of trying to modify it in-place. Note that the full (deep) copy is not always necessary in order to achieve copy-on-change semantics: it's enough (and often preferrable for performance reasons) to copy only the parts of the objects that need to be modified.

Assays has currently 3 implementations which are formalized by concrete subclasses SimpleListAssays, ShallowSimpleListAssays, and AssaysInEnv. ShallowSimpleListAssays is the default.

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AssaysInEnv is a *broken* alternative to ShallowSimpleListAssays that does NOT respect the *copy-on-change contract*. It is only provided for illustration purposes (see source file Assays-class.R for the details).

A little more detail about ShallowSimpleListAssays: a small reference class hierarchy (not exported from the **GenomicRanges** name space) defines a reference class ShallowData with a single field data of type ANY, and a derived class ShallowSimpleListAssays that specializes the type of data as SimpleList, and contains=c("ShallowData", "Assays"). The assays slot of a SummarizedExperiment object contains an instance of ShallowSimpleListAssays.

Author(s)

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See Also

- SummarizedExperiment objects.
- SimpleList objects in the S4Vectors package.

```
## DIRECT MANIPULATION OF Assays OBJECTS
## -----
m1 <- matrix(runif(24), ncol=3)</pre>
m2 <- matrix(runif(24), ncol=3)</pre>
a <- Assays(SimpleList(m1, m2))</pre>
а
as(a, "SimpleList")
length(a)
a[[2]]
dim(a)
b <- a[-4, 2]
length(b)
b[[2]]
dim(b)
names(a)
names(a) <- c("a1", "a2")
names(a)
a[["a2"]]
rbind(a, a)
cbind(a, a)
## COPY-ON-CHANGE CONTRACT
## ShallowSimpleListAssays objects have copy-on-change semantics but not
## AssaysInEnv objects. For example:
ssla <- as(SimpleList(m1, m2), "ShallowSimpleListAssays")</pre>
aie <- as(SimpleList(m1, m2), "AssaysInEnv")</pre>
```

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coverage-methods

Coverage of a RangedSummarizedExperiment object

Description

This man page documents the coverage method for RangedSummarizedExperiment objects.

Usage

Arguments

```
x A RangedSummarizedExperiment object.
shift, width, weight, method
See ?coverage in the GenomicRanges package.
```

Details

This method operates on the rowRanges component of the RangedSummarizedExperiment object, which can be a GenomicRanges or GRangesList object.

More precisely, on RangedSummarizedExperiment object x, coverage(x, ...) is equivalent to coverage(rowRanges(x), ...).

See ?coverage in the **GenomicRanges** package for the details of how coverage operates on a GenomicRanges or GRangesList object.

Value

See ?coverage in the GenomicRanges package.

See Also

- RangedSummarizedExperiment objects.
- The coverage man page in the GenomicRanges package where the coverage methods for GenomicRanges and GRangesList objects are documented.

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Examples

findOverlaps-methods Finding overlapping ranges in RangedSummarizedExperiment objects

Description

This man page documents the findOverlaps methods for RangedSummarizedExperiment objects.

RangedSummarizedExperiment objects also support countOverlaps, overlapsAny, and subsetByOverlaps thanks to the default methods defined in the **IRanges** package and to the findOverlaps methods defined in this package and documented below.

Usage

```
## S4 method for signature 'RangedSummarizedExperiment,Vector'
findOverlaps(query, subject,
    maxgap=-1L, minoverlap=0L,
    type=c("any", "start", "end", "within", "equal"),
    select=c("all", "first", "last", "arbitrary"),
    ignore.strand=FALSE)
## S4 method for signature 'Vector,RangedSummarizedExperiment'
findOverlaps(query, subject,
    maxgap=-1L, minoverlap=0L,
    type=c("any", "start", "end", "within", "equal"),
    select=c("all", "first", "last", "arbitrary"),
    ignore.strand=FALSE)
```

Arguments

```
query, subject One of these two arguments must be a RangedSummarizedExperiment object.

maxgap, minoverlap, type

See ?findOverlaps in the GenomicRanges package.

select, ignore.strand

See ?findOverlaps in the GenomicRanges package.
```

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Details

These methods operate on the rowRanges component of the RangedSummarizedExperiment object, which can be a GenomicRanges or GRangesList object.

More precisely, if any of the above functions is passed a RangedSummarizedExperiment object thru the query and/or subject argument, then it behaves as if rowRanges(query) and/or rowRanges(subject) had been passed instead.

See ?findOverlaps in the **GenomicRanges** package for the details of how findOverlaps and family operate on GenomicRanges and GRangesList objects.

Value

See ?findOverlaps in the GenomicRanges package.

See Also

- RangedSummarizedExperiment objects.
- The findOverlaps man page in the **GenomicRanges** package where the findOverlaps family of methods for GenomicRanges and GRangesList objects is documented.

Examples

inter-range-methods

Inter range transformations of a RangedSummarizedExperiment object

Description

This man page documents the *inter range transformations* that are supported on RangedSummarizedExperiment objects.

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Usage

```
## S4 method for signature 'RangedSummarizedExperiment'
isDisjoint(x, ignore.strand=FALSE)

## S4 method for signature 'RangedSummarizedExperiment'
disjointBins(x, ignore.strand=FALSE)
```

Arguments

```
x A RangedSummarizedExperiment object.

ignore.strand See ?isDisjoint in the GenomicRanges package.
```

Details

These transformations operate on the rowRanges component of the RangedSummarizedExperiment object, which can be a GenomicRanges or GRangesList object.

More precisely, any of the above functions performs the following transformation on RangedSummarizedExperiment object x:

```
f(rowRanges(x), ...)
```

where f is the name of the function and ... any additional arguments passed to it.

See ?isDisjoint in the **GenomicRanges** package for the details of how these transformations operate on a GenomicRanges or GRangesList object.

Value

See ?isDisjoint in the **GenomicRanges** package.

See Also

- RangedSummarizedExperiment objects.
- The isDisjoint man page in the **GenomicRanges** package where *inter range transformations* of a GenomicRanges or GRangesList object are documented.

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```
stopifnot(identical(bins0, disjointBins(rowRanges(rse0))))
bins1 <- disjointBins(rse1)
bins1
stopifnot(all(bins1 == bins1[1]))</pre>
```

intra-range-methods

Intra range transformations of a RangedSummarizedExperiment object

Description

This man page documents the *intra range transformations* that are supported on RangedSummarizedExperiment objects.

Usage

```
## S4 method for signature 'RangedSummarizedExperiment'
shift(x, shift=0L, use.names=TRUE)
## S4 method for signature 'RangedSummarizedExperiment'
narrow(x, start=NA, end=NA, width=NA, use.names=TRUE)
## S4 method for signature 'RangedSummarizedExperiment'
resize(x, width, fix="start", use.names=TRUE,
       ignore.strand=FALSE)
## S4 method for signature 'RangedSummarizedExperiment'
flank(x, width, start=TRUE, both=FALSE,
      use.names=TRUE, ignore.strand=FALSE)
## S4 method for signature 'RangedSummarizedExperiment'
promoters(x, upstream=2000, downstream=200)
## S4 method for signature 'RangedSummarizedExperiment'
restrict(x, start=NA, end=NA, keep.all.ranges=FALSE,
         use.names=TRUE)
## S4 method for signature 'RangedSummarizedExperiment'
trim(x, use.names=TRUE)
```

Arguments

```
x A RangedSummarizedExperiment object.
shift, use.names
See ?shift in the GenomicRanges package.
start, end, width, fix
See ?shift in the GenomicRanges package.
ignore.strand, both
See ?shift in the GenomicRanges package.
```

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```
upstream, downstream

See ?shift in the GenomicRanges package.

keep.all.ranges

See ?shift in the GenomicRanges package.
```

Details

These transformations operate on the rowRanges component of the RangedSummarizedExperiment object, which can be a GenomicRanges or GRangesList object.

More precisely, any of the above functions performs the following transformation on RangedSummarizedExperiment object x:

```
rowRanges(x) <- f(rowRanges(x), ...)</pre>
```

where f is the name of the function and ... any additional arguments passed to it.

See ?shift in the **GenomicRanges** package for the details of how these transformations operate on a GenomicRanges or GRangesList object.

See Also

- RangedSummarizedExperiment objects.
- The shift man page in the **GenomicRanges** package where *intra range transformations* of a GenomicRanges or GRangesList object are documented.

```
nrows <- 20; ncols <- 6
counts <- matrix(runif(nrows * ncols, 1, 1e4), nrows)</pre>
rowRanges <- GRanges(rep(c("chr1", "chr2"), c(5, 15)),</pre>
                      IRanges(sample(1000L, 20), width=100),
                      strand=Rle(c("+", "-"), c(12, 8)))
colData <- DataFrame(Treatment=rep(c("ChIP", "Input"), 3),</pre>
                      row.names=LETTERS[1:6])
rse0 <- SummarizedExperiment(assays=SimpleList(counts=counts),</pre>
                               rowRanges=rowRanges, colData=colData)
rse1 <- shift(rse0, 1)</pre>
stopifnot(identical(
  rowRanges(rse1),
  shift(rowRanges(rse0), 1)
))
se2 <- narrow(rse0, start=10, end=-15)
stopifnot(identical(
  rowRanges(se2),
  narrow(rowRanges(rse0), start=10, end=-15)
))
se3 <- resize(rse0, width=75)</pre>
stopifnot(identical(
  rowRanges(se3),
  resize(rowRanges(rse0), width=75)
se4 <- flank(rse0, width=20)</pre>
```

```
stopifnot(identical(
  rowRanges(se4),
  flank(rowRanges(rse0), width=20)
))
se5 <- restrict(rse0, start=200, end=700, keep.all.ranges=TRUE)</pre>
stopifnot(identical(
  rowRanges(se5),
  restrict(rowRanges(rse0), start=200, end=700, keep.all.ranges=TRUE)
))
```

 ${\tt make Summarized Experiment From Data Frame}$

Make a RangedSummarizedExperiment from a data.frame or DataFrame

Description

makeSummarizedExperimentFromDataFrame uses data.frame or DataFrame column names to create a GRanges object for the rowRanges of the resulting SummarizedExperiment object. It requires that non-range data columns be coercible into a numeric matrix for the SummarizedExperiment constructor. All columns that are not part of the row ranges attribute are assumed to be experiment data; thus, keeping metadata columns will not be supported. Note that this function only returns SummarizedExperiment objects with a single assay.

If metadata columns are to be kept, one can first construct the row ranges attribute by using the makeGRangesFromDataFrame function and subsequently creating the SummarizedExperiment.

Usage

```
makeSummarizedExperimentFromDataFrame(df,
                                     seginfo = NULL,
                                     starts.in.df.are.0based = FALSE)
```

Arguments

seqinfo

df A data frame or DataFrame object. If not, then the function first tries to turn df into a data frame with as.data.frame(df).

Additional arguments passed on to makeGRangesFromDataFrame

. . .

Either NULL, or a Seqinfo object, or a character vector of seqlevels, or a named numeric vector of sequence lengths. When not NULL, it must be compatible with the genomic ranges in df i.e. it must include at least the sequence levels represented in df.

starts.in.df.are.0based

TRUE or FALSE (the default). If TRUE, then the start positions of the genomic ranges in df are considered to be 0-based and are converted to 1-based in the returned GRanges object. This feature is intended to make it more convenient to handle input that contains data obtained from resources using the "0-based start" convention. A notorious example of such resource is the UCSC Table Browser (http://genome.ucsc.edu/cgi-bin/hgTables).

Value

A RangedSummarizedExperiment object with rowRanges and a single assay

Author(s)

M. Ramos

See Also

• makeGRangesFromDataFrame

Examples

 ${\tt make Summarized Experiment From Expression Set}$

Make a RangedSummarizedExperiment object from an ExpressionSet and vice-versa

Description

Coercion between RangedSummarizedExperiment and ExpressionSet is supported in both directions

For going from ExpressionSet to RangedSummarizedExperiment, the makeSummarizedExperimentFromExpressionSet function is also provided to let the user control how to map features to ranges.

Usage

Arguments

from An ExpressionSet object.

mapFun A function which takes an ExpressionSet object and returns a GRanges, or

GRangesList object which corresponds to the genomic ranges used in the ExpressionSet. The rownames of the returned GRanges are used to match the

featureNames of the ExpressionSet.

The naiveRangeMapper function is used by default.

... Additional arguments passed to mapFun.

txDbPackage A character string with the Transcript Database to use for the mapping.

key A character string with the Gene key to use for the mapping.

Value

makeSummarizedExperimentFromExpressionSet takes an ExpressionSet object as input and a range mapping function that maps the features to ranges. It then returns a RangedSummarizedExperiment object that corresponds to the input.

The range mapping functions return a GRanges object, with the rownames corresponding to the featureNames of the ExpressionSet object.

Author(s)

```
Jim Hester, james.f.hester@gmail.com
```

See Also

- RangedSummarizedExperiment objects.
- ExpressionSet objects in the Biobase package.
- TxDb objects in the GenomicFeatures package.

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```
example(RangedSummarizedExperiment) # to create 'rse'
rse
as(rse, "ExpressionSet")
```

nearest-methods

Finding the nearest range neighbor in RangedSummarizedExperiment objects

Description

This man page documents the nearest methods and family (i.e. precede, follow, distance, and distanceToNearest methods) for RangedSummarizedExperiment objects.

Usage

```
## S4 method for signature 'RangedSummarizedExperiment, ANY'
precede(x, subject, select=c("arbitrary", "all"),
        ignore.strand=FALSE)
## S4 method for signature 'ANY,RangedSummarizedExperiment'
precede(x, subject, select=c("arbitrary", "all"),
        ignore.strand=FALSE)
## S4 method for signature 'RangedSummarizedExperiment, ANY'
follow(x, subject, select=c("arbitrary", "all"),
        ignore.strand=FALSE)
## S4 method for signature 'ANY, RangedSummarizedExperiment'
follow(x, subject, select=c("arbitrary", "all"),
        ignore.strand=FALSE)
## S4 method for signature 'RangedSummarizedExperiment, ANY'
nearest(x, subject, select=c("arbitrary", "all"), ignore.strand=FALSE)
## S4 method for signature 'ANY,RangedSummarizedExperiment'
nearest(x, subject, select=c("arbitrary", "all"), ignore.strand=FALSE)
## S4 method for signature 'RangedSummarizedExperiment, ANY'
distance(x, y, ignore.strand=FALSE, ...)
## S4 method for signature 'ANY,RangedSummarizedExperiment'
distance(x, y, ignore.strand=FALSE, ...)
## S4 method for signature 'RangedSummarizedExperiment, ANY'
distanceToNearest(x, subject, ignore.strand=FALSE, ...)
## S4 method for signature 'ANY, RangedSummarizedExperiment'
distanceToNearest(x, subject, ignore.strand=FALSE, ...)
```

Arguments

```
x, subject One of these two arguments must be a RangedSummarizedExperiment object. select, ignore.strand
```

See ?nearest in the GenomicRanges package.

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y For the distance methods, one of x or y must be a RangedSummarizedExperiment object.

... Additional arguments for methods.

Details

These methods operate on the rowRanges component of the RangedSummarizedExperiment object, which can be a GenomicRanges or GRangesList object.

More precisely, if any of the above functions is passed a RangedSummarizedExperiment object thru the x, subject, and/or y argument, then it behaves as if rowRanges(x), rowRanges(subject), and/or rowRanges(y) had been passed instead.

See ?nearest in the **GenomicRanges** package for the details of how nearest and family operate on GenomicRanges and GRangesList objects.

Value

See ?nearest in the GenomicRanges package.

See Also

- RangedSummarizedExperiment objects.
- The nearest man page in the **GenomicRanges** package where the nearest family of methods for GenomicRanges and GRangesList objects is documented.

```
nrows <- 20; ncols <- 6
counts <- matrix(runif(nrows * ncols, 1, 1e4), nrows)</pre>
rowRanges <- GRanges(rep(c("chr1", "chr2"), c(5, 15)),</pre>
                      IRanges(sample(1000L, 20), width=100),
                      strand=Rle(c("+", "-"), c(12, 8)))
colData <- DataFrame(Treatment=rep(c("ChIP", "Input"), 3),</pre>
                      row.names=LETTERS[1:6])
rse0 <- SummarizedExperiment(assays=SimpleList(counts=counts),</pre>
                              rowRanges=rowRanges, colData=colData)
rse1 <- shift(rse0, 100)
res <- nearest(rse0, rse1)</pre>
stopifnot(identical(res, nearest(rowRanges(rse0), rowRanges(rse1))))
stopifnot(identical(res, nearest(rse0, rowRanges(rse1))))
stopifnot(identical(res, nearest(rowRanges(rse0), rse1)))
res <- nearest(rse0) # missing subject</pre>
stopifnot(identical(res, nearest(rowRanges(rse0))))
hits <- nearest(rse0, rse1, select="all")</pre>
hits
stopifnot(identical(
 hits,
  nearest(rowRanges(rse0), rowRanges(rse1), select="all")
stopifnot(identical(
  hits,
```

```
nearest(rse0, rowRanges(rse1), select="all")
))
stopifnot(identical(
  hits,
  nearest(rowRanges(rse0), rse1, select="all")
))
```

RangedSummarizedExperiment-class

RangedSummarizedExperiment objects

Description

The RangedSummarizedExperiment class is a matrix-like container where rows represent ranges of interest (as a GRanges or GRangesList object) and columns represent samples (with sample data summarized as a DataFrame). A RangedSummarizedExperiment contains one or more assays, each represented by a matrix-like object of numeric or other mode.

RangedSummarizedExperiment is a subclass of SummarizedExperiment and, as such, all the methods documented in ?SummarizedExperiment also work on a RangedSummarizedExperiment object. The methods documented below are additional methods that are specific to RangedSummarizedExperiment objects.

Usage

```
## Constructor
SummarizedExperiment(assays, ...)
## S4 method for signature 'SimpleList'
SummarizedExperiment(assays, rowData=NULL, rowRanges=GRangesList(),
    colData=DataFrame(), metadata=list())
## S4 method for signature 'ANY'
SummarizedExperiment(assays, ...)
## S4 method for signature 'list'
SummarizedExperiment(assays, ...)
## S4 method for signature 'missing'
SummarizedExperiment(assays, ...)
## Accessors
rowRanges(x, ...)
rowRanges(x, ...) <- value</pre>
## Subsetting
## S4 method for signature 'RangedSummarizedExperiment'
subset(x, subset, select, ...)
## rowRanges access
## see 'GRanges compatibility', below
```

Arguments

A list or SimpleList of matrix-like elements, or a matrix-like object. All assays elements of the list must have the same dimensions, and dimension names (if present) must be consistent across elements and with the row names of rowRanges and colData. rowData A DataFrame object describing the rows. Row names, if present, become the row names of the SummarizedExperiment object. The number of rows of the DataFrame must equal the number of rows of the matrices in assays. A GRanges or GRangesList object describing the ranges of interest. Names, rowRanges if present, become the row names of the SummarizedExperiment object. The length of the GRanges or GRangesList must equal the number of rows of the matrices in assays. If rowRanges is missing, a SummarizedExperiment instance is returned. colData An optional DataFrame describing the samples. Row names, if present, become the column names of the RangedSummarizedExperiment. metadata An optional list of arbitrary content describing the overall experiment. For SummarizedExperiment, S4 methods list and matrix, arguments identical to those of the SimpleList method. For rowRanges, ignored. A RangedSummarizedExperiment object. The rowRanges setter will also accept Х a SummarizedExperiment object and will first coerce it to RangedSummarized-Experiment before it sets value on it. A GRanges or GRangesList object. value subset An expression which, when evaluated in the context of rowRanges(x), is a logical vector indicating elements or rows to keep: missing values are taken as false. select An expression which, when evaluated in the context of colData(x), is a logical vector indicating elements or rows to keep: missing values are taken as false.

Details

The rows of a RangedSummarizedExperiment object represent ranges (in genomic coordinates) of interest. The ranges of interest are described by a GRanges or a GRangesList object, accessible using the rowRanges function, described below. The GRanges and GRangesList classes contains sequence (e.g., chromosome) name, genomic coordinates, and strand information. Each range can be annotated with additional data; this data might be used to describe the range or to summarize results (e.g., statistics of differential abundance) relevant to the range. Rows may or may not have row names; they often will not.

Constructor

RangedSummarizedExperiment instances are constructed using the SummarizedExperiment function with arguments outlined above.

Accessors

In the following code snippets, x is a RangedSummarizedExperiment object.

rowRanges(x), rowRanges(x) <- value: Get or set the row data. value is a GenomicRanges object. Row names of value must be NULL or consistent with the existing row names of x.

GRanges compatibility (rowRanges access)

Many GRanges and GRangesList operations are supported on RangedSummarizedExperiment objects, using rowRanges.

Supported operations include: pcompare, duplicated, end, end<-, granges, is.unsorted, match, mcols, mcols<-, order, ranges, ranges<-, rank, seqinfo, seqinfo<-, seqnames, sort, start, start<-, strand, strand<-, width, width<-.

See also ?shift, ?isDisjoint, ?coverage, ?findOverlaps, and ?nearest for more *GRanges compatibility methods*.

Not all GRanges operations are supported, because they do not make sense for RangedSummarizedExperiment objects (e.g., length, name, as.data.frame, c, splitAsList), involve non-trivial combination or splitting of rows (e.g., disjoin, gaps, reduce, unique), or have not yet been implemented (Ops, map, window, window<-).

Subsetting

In the code snippets below, x is a RangedSummarizedExperiment object.

```
subset(x, subset, select): Create a subset of x using an expression subset referring to columns
    of rowRanges(x) (including 'seqnames', 'start', 'end', 'width', 'strand', and names(rowData(x)))
    and / or select referring to column names of colData(x).
```

Extension

RangedSummarizedExperiment is implemented as an S4 class, and can be extended in the usual way, using contains="RangedSummarizedExperiment" in the new class definition.

Author(s)

Martin Morgan, mtmorgan@fhcrc.org

See Also

- SummarizedExperiment objects.
- shift, isDisjoint, coverage, findOverlaps, and nearest for more GRanges compatibility methods.
- GRanges objects in the GenomicRanges package.

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```
head(assay(rse))
assays(rse) <- endoapply(assays(rse), asinh)</pre>
head(assay(rse))
rowRanges(rse)
rowData(rse) # same as 'mcols(rowRanges(rse))'
colData(rse)
rse[, rse$Treatment == "ChIP"]
## cbind() combines objects with the same ranges but different samples:
rse1 <- rse
rse2 <- rse1[,1:3]
colnames(rse2) <- letters[1:ncol(rse2)]</pre>
cmb1 <- cbind(rse1, rse2)</pre>
dim(cmb1)
dimnames(cmb1)
## rbind() combines objects with the same samples but different ranges:
rse1 <- rse
rse2 <- rse1[1:50,]
rownames(rse2) <- letters[1:nrow(rse2)]</pre>
cmb2 <- rbind(rse1, rse2)</pre>
dim(cmb2)
dimnames(cmb2)
## Coercion to/from SummarizedExperiment:
se0 <- as(rse, "SummarizedExperiment")</pre>
se0
as(se0, "RangedSummarizedExperiment")
## Setting rowRanges on a SummarizedExperiment object turns it into a
## RangedSummarizedExperiment object:
se <- se0
rowRanges(se) <- rowRanges</pre>
se # RangedSummarizedExperiment
## Sanity checks:
stopifnot(identical(assays(se0), assays(rse)))
stopifnot(identical(dim(se0), dim(rse)))
stopifnot(identical(dimnames(se0), dimnames(rse)))
stopifnot(identical(rowData(se0), rowData(rse)))
stopifnot(identical(colData(se0), colData(rse)))
```

readKallisto

Input kallisto or kallisto bootstrap results.

Description

readKallisto inputs several kallisto output files into a single SummarizedExperiment instance, with rows corresponding to estimated transcript abundance and columns to samples. readKallistoBootstrap inputs kallisto bootstrap replicates of a single sample into a matrix of transcript x bootstrap abundance estimates.

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Usage

```
readKallisto(files,
    json = file.path(dirname(files), "run_info.json"),
    h5 = any(grepl("\\.h5$", files)), what = KALLISTO_ASSAYS,
    as = c("SummarizedExperiment", "list", "matrix"))
readKallistoBootstrap(file, i, j)
```

Arguments

files	character() paths to kallisto 'abundance.tsv' output files. The assumption is that files are organized in the way implied by kallisto, with each sample in a distinct directory, and the directory containing files abundance.tsv, run_info.json, and perhaps abundance.h5.
json	character() vector of the same length as files specifying the location of JSON files produced by kallisto and containing information on the run. The default assumes that json files are in the same directory as the corresponding abundance file.
h5	character() vector of the same length as files specifying the location of HDF5 files produced by kallisto and containing bootstrap estimates. The default assumes that HDF5 files are in the same directory as the corresponding abundance file.
what	$character()\ vector\ of\ kallisto\ per-sample\ outputs\ to\ be\ input.\ See\ KALLISTO_ASSAYS\ for\ available\ values.$
as	character(1) specifying the output format. See Value for additional detail.
file	character(1) path to a single HDF5 output file.
i, j	integer() vector of row (i) and column (j) indexes to input.

Value

A SummarizedExperiment, list, or matrix, depending on the value of argument as; by default a SummarizedExperiment. The as="SummarizedExperiment" rowData(se) the length of each transcript; colData(se) includes summary information on each sample, including the number of targets and bootstraps, the kallisto and index version, the start time and operating system call used to create the file. assays() contains one or more transcript x sample matrices of parameters estimated by kallisto (see KALLISTO_ASSAYS).

as="list" return value contains information simillar to SummarizedExperiment with row, column and assay data as elements of the list without coordination of row and column annotations into an integrated data container. as="matrix" returns the specified assay as a simple *R* matrix.

Author(s)

Martin Morgan martin.morgan@roswellpark.org

References

http://pachterlab.github.io/kallisto software for quantifying transcript abundance.

Examples

```
outputs <- system.file(package="SummarizedExperiment", "extdata",</pre>
    "kallisto")
files <- dir(outputs, pattern="abundance.tsv", full=TRUE, recursive=TRUE)
stopifnot(all(file.exists(files)))
## default: input 'est_counts'
(se <- readKallisto(files, as="SummarizedExperiment"))</pre>
str(readKallisto(files, as="list"))
str(readKallisto(files, as="matrix"))
## available assays
KALLISTO_ASSAYS
## one or more assay
readKallisto(files, what=c("tpm", "eff_length"))
## alternatively: read hdf5 files
files <- sub(".tsv", ".h5", files, fixed=TRUE)</pre>
readKallisto(files)
## input all bootstraps
xx <- readKallistoBootstrap(files[1])</pre>
ridx <- head(which(rowSums(xx) != 0), 3)</pre>
cidx <- c(1:5, 96:100)
xx[ridx, cidx]
## selective input of rows (transcripts) and/or bootstraps
readKallistoBootstrap(files[1], i=c(ridx, rev(ridx)), j=cidx)
```

saveHDF5SummarizedExperiment

Save/load a HDF5-based SummarizedExperiment object

Description

saveHDF5SummarizedExperiment and loadHDF5SummarizedExperiment can be used to save/load a HDF5-based SummarizedExperiment object to/from disk.

Usage

```
save HDF5 Summarized Experiment (x, dir="my_h5_se", replace=FALSE, chunk\_dim=NULL, level=NULL, verbose=FALSE) \\ load HDF5 Summarized Experiment (dir="my_h5_se")
```

tent of the existing directory will be lost!

Arguments

x	A SummarizedExperiment object.
dir	The path (as a single string) to the directory where to save the HDF5-based SummarizedExperiment object or to load it from. When saving, the directory will be created so should not already exist, unless replace is set to TRUE.
replace	If directory dir already exists, should it be replaced with a new one? The con-

```
chunk_dim, level
```

The dimensions of the chunks and the compression level to use for writting the assay data to disk. Passed to the internal calls to HDF5Array::writeHDF5Array. See ?HDF5Array::writeHDF5Array for more information.

verbose

Set to TRUE to make the function display progress.

Details

These functions use functionalities from the **rhdf5** and **HDF5Array** packages internally and so require these packages to be installed.

saveHDF5SummarizedExperiment creates the directory specified thru the dir argument and then populates it with the HDF5 datasets (one per assay in x) plus a serialized version of x that contains pointers to these datasets. This directory provides a self-contained HDF5-based representation of x that can then be loaded back in R with loadHDF5SummarizedExperiment. Note that this directory is *relocatable* i.e. it can be moved (or copied) to a different place, on the same or a different computer, before calling loadHDF5SummarizedExperiment on it. For convenient sharing with collaborators, it is suggested to turn it into a tarball (with Unix command tar), or zip file, before the transfer. Please keep in mind that saveHDF5SummarizedExperiment and loadHDF5SummarizedExperiment don't know how to produce/read tarballs or zip files at the moment, so the process of packaging/extracting the tarball or zip file is entirely the user responsibility. It is typically done from outside R.

Finally please note that, depending on the size of the data to write to disk and the performance of the disk, saveHDF5SummarizedExperiment can take a long time to complete. Use verbose=TRUE to see its progress.

loadHDF5SummarizedExperiment is generally very fast, even if the assay data is big, because all the assays in the returned object are HDF5Array objects pointing to the on-disk HDF5 datasets located in dir. HDF5Array objects are typically light-weight in memory.

Value

saveHDF5SummarizedExperiment returns an invisible SummarizedExperiment object where all the assays are HDF5Array objects pointing to the HDF5 datasets saved in dir. It's in fact the same obect as the object that would be returned by calling loadHDF5SummarizedExperiment on dir.

Author(s)

Hervé Pagès

See Also

- SummarizedExperiment and RangedSummarizedExperiment objects.
- HDF5Array objects in the HDF5Array package.
- The writeHDF5Array function in the **HDF5Array** package, which saveHDF5SummarizedExperiment uses internally to write the assay data to disk.

```
colData=colData)
se0
## Save 'se0' as an HDF5-based SummarizedExperiment object:
dir <- sub("file", "h5_se0_", tempfile())</pre>
h5_se0 <- saveHDF5SummarizedExperiment(se0, dir)</pre>
h5 se0
assay(h5_se0, withDimnames=FALSE) # HDF5Matrix object
h5_se0b <- loadHDF5SummarizedExperiment(dir)</pre>
assay(h5_se0b, withDimnames=FALSE) # HDF5Matrix object
## Sanity checks:
stopifnot(is(assay(h5_se0, withDimnames=FALSE), "HDF5Matrix"))
stopifnot(all(DelayedArray(assay(se0)) == assay(h5_se0)))
stopifnot(is(assay(h5_se0b, withDimnames=FALSE), "HDF5Matrix"))
stopifnot(all(DelayedArray(assay(se0)) == assay(h5_se0b)))
## More sanity checks
## -----
## Make a copy of directory 'dir':
somedir <- sub("file", "somedir", tempfile())</pre>
dir.create(somedir)
file.copy(dir, somedir, recursive=TRUE)
dir2 <- list.files(somedir, full.names=TRUE)</pre>
## 'dir2' contains a copy of 'dir'. Call loadHDF5SummarizedExperiment()
## on it.
h5_se0c <- loadHDF5SummarizedExperiment(dir2)</pre>
stopifnot(is(assay(h5_se0c, withDimnames=FALSE), "HDF5Matrix"))
stopifnot(all(DelayedArray(assay(se0)) == assay(h5_se0c)))
```

SummarizedExperiment-class

SummarizedExperiment objects

Description

The SummarizedExperiment class is a matrix-like container where rows represent features of interest (e.g. genes, transcripts, exons, etc...) and columns represent samples (with sample data summarized as a DataFrame). A SummarizedExperiment object contains one or more assays, each represented by a matrix-like object of numeric or other mode.

Note that SummarizedExperiment is the parent of the RangedSummarizedExperiment class which means that all the methods documented below also work on a RangedSummarizedExperiment object.

Usage

```
## Constructor
# See ?RangedSummarizedExperiment for the constructor function.
## Accessors
assayNames(x, ...)
assayNames(x, ...) \leftarrow value
assays(x, ..., withDimnames=TRUE)
assays(x, ..., withDimnames=TRUE) <- value
assay(x, i, ...)
assay(x, i, ...) \leftarrow value
rowData(x, ...)
rowData(x, ...) <- value</pre>
colData(x, ...)
colData(x, ...) <- value
#dim(x)
#dimnames(x)
\#dimnames(x) \leftarrow value
## Quick colData access
## S4 method for signature 'SummarizedExperiment'
## S4 replacement method for signature 'SummarizedExperiment'
x$name <- value
## S4 method for signature 'SummarizedExperiment, ANY, missing'
x[[i, j, ...]]
## S4 replacement method for signature 'SummarizedExperiment,ANY,missing'
x[[i, j, \ldots]] \leftarrow value
## Subsetting
## S4 method for signature 'SummarizedExperiment'
x[i, j, ..., drop=TRUE]
## S4 replacement method for signature 'SummarizedExperiment,ANY,ANY,SummarizedExperiment'
x[i, j] \leftarrow value
## Combining
## S4 method for signature 'SummarizedExperiment'
cbind(..., deparse.level=1)
## S4 method for signature 'SummarizedExperiment'
rbind(..., deparse.level=1)
## On-disk realization
## S4 method for signature 'SummarizedExperiment'
realize(x)
```

Arguments

A SummarizedExperiment object.

... For assay, ... may contain withDimnames, which is forwarded to assays.

For rowData, arguments passed thru . . . are forwarded to mcols.

For cbind, rbind, ... contains SummarizedExperiment objects to be com-

bined.

For other accessors, ignored.

i, j For assay, assay<-, i is an integer or numeric scalar; see 'Details' for addi-

tional constraints.

For [,SummarizedExperiment, [,SummarizedExperiment<-, i, j are subscripts that can act to subset the rows and columns of x, that is the matrix

elements of assays.

For [[,SummarizedExperiment, [[<-,SummarizedExperiment, i is a scalar α]

index (e.g., character(1) or integer(1)) into a column of colData.

name A symbol representing the name of a column of colData.

withDimnames A logical(1), indicating whether dimnames should be applied to extracted

assay elements. Setting withDimnames=FALSE increases the speed and memory efficiency with which assays are extracted. withDimnames=TRUE in the getter assays<- allows efficient complex assignments (e.g., updating names of assays, names(assays(x, withDimnames=FALSE)) = ... is more efficient than names(assays(x)) = ...); it does not influence actual assignment of

dimnames to assays.

drop A logical(1), ignored by these methods.

value An object of a class specified in the S4 method signature or as outlined in 'De-

tails'.

deparse.level See ?base::cbind for a description of this argument.

Details

The SummarizedExperiment class is meant for numeric and other data types derived from a sequencing experiment. The structure is rectangular like a matrix, but with additional annotations on the rows and columns, and with the possibility to manage several assays simultaneously.

The rows of a SummarizedExperiment object represent features of interest. Information about these features is stored in a DataFrame object, accessible using the function rowData. The DataFrame must have as many rows as there are rows in the SummarizedExperiment object, with each row of the DataFrame providing information on the feature in the corresponding row of the SummarizedExperiment object. Columns of the DataFrame represent different attributes of the features of interest, e.g., gene or transcript IDs, etc.

Each column of a SummarizedExperiment object represents a sample. Information about the samples are stored in a DataFrame, accessible using the function colData, described below. The DataFrame must have as many rows as there are columns in the SummarizedExperiment object, with each row of the DataFrame providing information on the sample in the corresponding column of the SummarizedExperiment object. Columns of the DataFrame represent different sample attributes, e.g., tissue of origin, etc. Columns of the DataFrame can themselves be annotated (via the mcols function). Column names typically provide a short identifier unique to each sample.

A SummarizedExperiment object can also contain information about the overall experiment, for instance the lab in which it was conducted, the publications with which it is associated, etc. This information is stored as a list object, accessible using the metadata function. The form of the data associated with the experiment is left to the discretion of the user.

The SummarizedExperiment container is appropriate for matrix-like data. The data are accessed using the assays function, described below. This returns a SimpleList object. Each element of

val

the list must itself be a matrix (of any mode) and must have dimensions that are the same as the dimensions of the SummarizedExperiment in which they are stored. Row and column names of each matrix must either be NULL or match those of the SummarizedExperiment during construction. It is convenient for the elements of SimpleList of assays to be named.

Constructor

SummarizedExperiment instances are constructed using the SummarizedExperiment function documented in ?RangedSummarizedExperiment.

Accessors

In the following code snippets, x is a SummarizedExperiment object.

- assays(x), assays(x) <- value: Get or set the assays. value is a list or SimpleList, each element of which is a matrix with the same dimensions as x.
- assay(x, i), assay(x, i) <- value: A convenient alternative (to assays(x)[[i]], assays(x)[[i]] <- to get or set the ith (default first) assay element. value must be a matrix of the same dimension as x, and with dimension names NULL or consistent with those of x.
- assayNames(x), assayNames(x) <- value: Get or set the names of assay() elements.
- rowData(x), rowData(x) <- value: Get or set the row data. value is a DataFrame object. Row names of value must be NULL or consistent with the existing row names of x.
- colData(x), colData(x) <- value: Get or set the column data. value is a DataFrame object. Row names of value must be NULL or consistent with the existing column names of x.
- metadata(x), metadata(x) <- value: Get or set the experiment data. value is a list with arbitrary content.
- dim(x): Get the dimensions (features of interest x samples) of the SummarizedExperiment.
- dimnames(x), dimnames(x) <- value: Get or set the dimension names. value is usually a list of length 2, containing elements that are either NULL or vectors of appropriate length for the corresponding dimension. value can be NULL, which removes dimension names. This method implies that rownames, rownames<-, colnames, and colnames<- are all available.

Subsetting

In the code snippets below, x is a SummarizedExperiment object.

x[i,j], x[i,j] <- value: Create or replace a subset of x. i, j can be numeric, logical, character, or missing. value must be a SummarizedExperiment object with dimensions, dimension names, and assay elements consistent with the subset x[i,j] being replaced.

Additional subsetting accessors provide convenient access to colData columns

```
x$name, x$name <- value Access or replace column name in x.
x[[i, ...]], x[[i, ...]] <- value Access or replace column i in x.</pre>
```

Combining

In the code snippets below, ... are SummarizedExperiment objects to be combined.

cbind(...): cbind combines objects with the same features of interest but different samples
 (columns in assays). The colnames in colData(SummarizedExperiment) must match or
 an error is thrown. Duplicate columns of rowData(SummarizedExperiment) must contain
 the same data.

Data in assays are combined by name matching; if all assay names are NULL matching is by position. A mixture of names and NULL throws an error.

metadata from all objects are combined into a list with no name checking.

rbind(...): rbind combines objects with the same samples but different features of interest (rows in assays). The colnames in rowData(SummarizedExperiment) must match or an error is thrown. Duplicate columns of colData(SummarizedExperiment) must contain the same data.

Data in assays are combined by name matching; if all assay names are NULL matching is by position. A mixture of names and NULL throws an error.

metadata from all objects are combined into a list with no name checking.

Implementation and Extension

This section contains advanced material meant for package developers.

SummarizedExperiment is implemented as an S4 class, and can be extended in the usual way, using contains="SummarizedExperiment" in the new class definition.

In addition, the representation of the assays slot of SummarizedExperiment is as a virtual class Assays. This allows derived classes (contains="Assays") to easily implement alternative requirements for the assays, e.g., backed by file-based storage like NetCDF or the ff package, while re-using the existing SummarizedExperiment class without modification. See Assays for more information.

The current assays slot is implemented as a reference class that has copy-on-change semantics. This means that modifying non-assay slots does not copy the (large) assay data, and at the same time the user is not surprised by reference-based semantics. Updates to non-assay slots are very fast; updating the assays slot itself can be 5x or more faster than with an S4 instance in the slot. One useful technique when working with assay or assays function is use of the withDimnames=FALSE argument, which benefits speed and memory use by not copying dimnames from the row- and colData elements to each assay.

Author(s)

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See Also

- RangedSummarizedExperiment objects.
- DataFrame, SimpleList, and Annotated objects in the **S4Vectors** package.
- The metadata and mcols accessors in the **S4Vectors** package.
- saveHDF5SummarizedExperiment and loadHDF5SummarizedExperiment for saving/loading a HDF5-based SummarizedExperiment object to/from disk.
- The realize generic function in the **DelayedArray** package for more information about ondisk realization of objects carrying delayed operations.

```
nrows <- 200; ncols <- 6
counts <- matrix(runif(nrows * ncols, 1, 1e4), nrows)</pre>
colData <- DataFrame(Treatment=rep(c("ChIP", "Input"), 3),</pre>
                   row.names=LETTERS[1:6])
se0 <- SummarizedExperiment(assays=SimpleList(counts=counts),</pre>
                          colData=colData)
se0
dim(se0)
dimnames(se0)
assayNames(se0)
head(assay(se0))
assays(se0) <- \ endoapply(assays(se0), \ asinh)
head(assay(se0))
rowData(se0)
colData(se0)
se0[, se0$Treatment == "ChIP"]
## cbind() combines objects with the same features of interest
## but different samples:
se1 <- se0
se2 <- se1[,1:3]
colnames(se2) <- letters[1:ncol(se2)]</pre>
cmb1 <- cbind(se1, se2)</pre>
dim(cmb1)
dimnames(cmb1)
## rbind() combines objects with the same samples but different
## features of interest:
se1 <- se0
se2 <- se1[1:50,]
rownames(se2) <- letters[1:nrow(se2)]</pre>
cmb2 <- rbind(se1, se2)</pre>
dim(cmb2)
dimnames(cmb2)
## -----
## ON-DISK REALIZATION
## -----
setRealizationBackend("HDF5Array")
cmb3 <- realize(cmb2)</pre>
assay(cmb3, withDimnames=FALSE) \# an HDF5Matrix object
```

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