Package ‘SummarizedExperiment’

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Title SummarizedExperiment container

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.

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Assays-class

Description

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

SimpleListAssays and ShallowSimpleListAssays are concrete subclasses of Assays with the latter
being currently the default implementation of Assays objects. Other implementations (e.g. disk-
based) 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 Sim-
pleList 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 performing 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 preferable 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 SimpleList-
Assays, ShallowSimpleListAssays, and AssaysInEnv. ShallowSimpleListAssays is the default.
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)

Martin Morgan, mtmorgan@fhcrc.org

See Also

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

Examples

```r
## ---------------------------------------------------------------------
## DIRECT MANIPULATION OF Assays OBJECTS
## ---------------------------------------------------------------------
m1 <- matrix(runif(24), ncol=3)
m2 <- matrix(runif(24), ncol=3)
a <- Assays(SimpleList(m1, m2))
a
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")
aie <- as(SimpleList(m1, m2), "AssaysInEnv")
```
## No names on 'ssl'a' and 'aie':

```r
names(ssl)
names(aie)
```

```r
ssl2 <- ssl
aie2 <- aie
names(ssl2) <- names(aie2) <- c("A1", "A2")
```

```r
names(ssl)  # still NULL (as expected)
names(aie)  # changed! (because the names<-,AssaysInEnv method is not # implemented in a way that respects the copy-on-change # contract)
```

---

**Coverage of a RangedSummarizedExperiment object**

### Description

This man page documents the `coverage` method for `RangedSummarizedExperiment` objects.

### Usage

```r
## S4 method for signature 'RangedSummarizedExperiment'
coverage(x, shift=0L, width=NULL, weight=1L,
  method=c("auto", "sort", "hash"))
```

### 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, for a `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.
**Examples**

```r
nrows <- 20; ncols <- 6
counts <- matrix(runif(nrows * ncols, 1, 1e4), nrows)
rowRanges <- GRanges(rep(c("chr1", "chr2"), c(5, 15)),
  IRanges(sample(1000L, 20), width=100),
  strand=Rle(c("+", "-"), c(12, 8)),
  seqlengths=c(chr1=1800, chr2=1300))
colData <- DataFrame(Treatment=rep(c("ChIP", "Input"), 3),
  row.names=LETTERS[1:6])
rse <- SummarizedExperiment(assays=SimpleList(counts=counts),
  rowRanges=rowRanges, colData=colData)

cvg <- coverage(rse)
cvg
stopifnot(identical(cvg, coverage(rowRanges(rse))))
```

---

**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**

```r
## S4 method for signature 'RangedSummarizedExperiment,Vector'
findOverlaps(query, subject,
  maxgap=0L, minoverlap=1L,
  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=0L, minoverlap=1L,
  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.
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

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

hits <- findOverlaps(rse0, rse1)
hits
stopifnot(identical(hits, findOverlaps(rowRanges(rse0), rowRanges(rse1))))
stopifnot(identical(hits, findOverlaps(rse0, rowRanges(rse1))))
stopifnot(identical(hits, findOverlaps(rowRanges(rse0), rse1)))
```

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.
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`:

\[ f(\text{rowRanges}(x), \ldots) \]

where `f` is the name of the function and \ldots 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.

Examples

```r
nrows <- 20; ncols <- 6
counts <- matrix(runif(nrows * ncols, 1, 1e4), nrows)
rowRanges <- GRanges(rep(c("chr1", "chr2"), c(5, 15)),
                      IRanges(sample(1000L, 20), width=100),
                      strand=Rle(c("+", "-"), c(12, 8)))
colData <- DataFrame(Treatment=rep(c("ChIP", "Input"), 3),
                      row.names=LETTERS[1:6])
rse0 <- SummarizedExperiment(assays=SimpleList(counts=counts),
                             rowRanges=rowRanges, colData=colData)
rse1 <- shift(rse0, 99*start(rse0))
isDisjoint(rse0) # FALSE

isDisjoint(rse1) # TRUE

bins0 <- disjointBins(rse0)
bins0
```
Intra range transformations of a RangedSummarizedExperiment object

Description

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

Usage

```r
## 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.
intra-range-methods

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:

\[
\text{rowRanges}(x) \leftarrow f(\text{rowRanges}(x), \ldots)
\]

where \( f \) is the name of the function and \( \ldots \) 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.

Examples

```r
nrows <- 20; ncols <- 6
counts <- matrix(runif(nrows * ncols, 1, 1e4), nrows)
rowRanges <- GRanges(rep(c("chr1", "chr2"), c(5, 15)),
                     IRanges(sample(1000L, 20), width=100),
                     strand=Rle(c("+", "-"), c(12, 8)))
colData <- DataFrame(Treatment=rep(c("ChIP", "Input"), 3),
                     row.names=LETTERS[1:6])
rse0 <- SummarizedExperiment(assays=SimpleList(counts=counts),
                              rowRanges=rowRanges, colData=colData)

rse1 <- shift(rse0, 1)
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)
stopifnot(identical(
    rowRanges(se3),
    resize(rowRanges(rse0), width=75)
))

se4 <- flank(rse0, width=20)
```
stopifnot(identical(
  rowRanges(se4),
  flank(rowRanges(rse0), width=20)
))

se5 <- restrict(rse0, start=200, end=700, keep.all.ranges=TRUE)
stopifnot(identical(
  rowRanges(se5),
  restrict(rowRanges(rse0), start=200, end=700, keep.all.ranges=TRUE)
))

---

makeSummarizedExperimentFromDataFrame

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

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

Arguments

- `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`
- `seqinfo` 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).
makeSummarizedExperimentFromExpressionSet

Value

A RangedSummarizedExperiment object with rowRanges and a single assay

Author(s)

M. Ramos

See Also

• makeGRangesFromDataFrame

Examples

## BASIC EXAMPLES

# Note that rownames of the data.frame are also rownames of the result
df <- data.frame(chr="chr2", start = 11:15, end = 12:16,
                 strand = c("+", "-", "+", "+", "."), expr0 = 3:7,
                 expr1 = 8:12, expr2 = 12:16,
                 row.names = paste0("GENE", letters[5:1]))

df

exRSE <- makeSummarizedExperimentFromDataFrame(df)
exRSE

assay(exRSE)

rowRanges(exRSE)

makeSummarizedExperimentFromExpressionSet

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

makeSummarizedExperimentFromExpressionSet(from,
                                           mapFun=naiveRangeMapper,
                                           ...)

## range mapping functions
naiveRangeMapper(from)
probeRangeMapper(from)
geneRangeMapper(txDbPackage, key = "ENTREZID")
makeSummarizedExperimentFromExpressionSet

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.hestergmail.com

See Also

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

Examples

## GOING FROM ExpressionSet TO RangedSummarizedExperiment
```r
data(sample.ExpressionSet, package="Biobase")

# 2 equivalent ways of doing the naive coercion
makeSummarizedExperimentFromExpressionSet(sample.ExpressionSet)
as(sample.ExpressionSet, "RangedSummarizedExperiment")

# using probe range mapper
makeSummarizedExperimentFromExpressionSet(sample.ExpressionSet, probeRangeMapper)

# using the gene range mapper
makeSummarizedExperimentFromExpressionSet(sample.ExpressionSet, geneRangeMapper("TxDb.Hsapiens.UCSC.hg19.knownGene"))
```

## GOING FROM RangedSummarizedExperiment TO ExpressionSet
```r
```
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.

y
For the distance methods, one of x or y must be a RangedSummarizedExperi-
ment 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.

Examples

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

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

```r
## 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

```r
rowRanges(x, ...)
rowRanges(x, ...) <- value
```

## Subsetting

```r
## S4 method for signature 'RangedSummarizedExperiment'
subset(x, subset, select, ...)
```

## rowRanges access

```r
## see 'GRanges compatibility', below
```

Arguments

- **assays**: A list or SimpleList of matrix-like elements, or a matrix-like object. All 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.

**rowRanges**
A GRanges or GRangesList object describing the ranges of interest. Names, 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.

**x**
A RangedSummarizedExperiment object. The rowRanges setter will also accept a SummarizedExperiment object and will first coerce it to RangedSummarizedExperiment before it sets value on it.

**value**
A GRanges or GRangesList object.

**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 contain 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.

```r
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.

Examples

nrows <- 200; ncols <- 6
counts <- matrix(runif(nrows * ncols, 1, 1e4), nrows)
rowRanges <- GRanges(rep(c("chr1", "chr2"), c(50, 150)),
IRanges(floor(runif(200, 1e5, 1e6)), width=100),
strand=sample(c("+", "-"), 200, TRUE),
feature_id=sprintf("ID%03d", 1:200))
colData <- DataFrame(Treatment=rep(c("ChIP", "Input"), 3),
row.names=LETTERS[1:6])
rse <- SummarizedExperiment(assays=SimpleList(counts=counts),
rowRanges=rowRanges, colData=colData)
rse
dim(rse)
dimnames(rse)
assayNames(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.
readKallisto

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 similar 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

```r
outputs <- system.file(package="SummarizedExperiment", "extdata", 
"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"))
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)
readKallisto(files)

## input all bootstraps
xx <- readKallistoBootstrap(files[1])
ridx <- head(which(rowSums(xx) != 0), 3)
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**

```r
saveHDF5SummarizedExperiment(x, dir="my_h5_se", replace=FALSE, 
chunk_dim=NULL, level=NULL, verbose=FALSE)
loadHDF5SummarizedExperiment(dir="my_h5_se")
```

**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 content of the existing directory will be lost!
saveHDF5SummarizedExperiment

chunk_dim, level
The dimensions of the chunks and the compression level to use for writing 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 con-
tains 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 mo-
ment, 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
object 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.

Examples
nrows <- 200; ncols <- 6
counts <- matrix(runif(nrows * ncols, 1, 1e4), nrows)
colData <- DataFrame(Treatment=rep(c("ChIP", "Input"), 3),
                      row.names=LETTERS[1:6])
se0 <- SummarizedExperiment(assays=SimpleList(counts=counts),
                          colData=colData)
## Save 'se0' as an HDF5-based SummarizedExperiment object:

dir <- sub("file", "h5_se0_", tempfile())
se0 <- saveHDF5SummarizedExperiment(se0, dir)

## Sanity checks:
stopifnot(is(assay(h5_se0, withDimnames=FALSE), "HDF5Matrix"))
stopifnot(all(DelayedArray(assay(se0)) == assay(h5_se0)))

## More sanity checks

## Make a copy of directory 'dir':
somedir <- sub("file", "somedir", tempfile())
dir.create(somedir)
file.copy(dir, somedir, recursive=TRUE)
dir2 <- list.files(somedir, full.names=TRUE)

## 'dir2' contains a copy of 'dir'. Call loadHDF5SummarizedExperiment() on it.

## SummarizedExperiment-class

### 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, ...) <- value  
assays(x, ..., withDimnames=TRUE)  
assays(x, ..., withDimnames=TRUE) <- value  
assay(x, i, ...)  
assay(x, i, ...) <- value  
rowData(x, ...)  
rowData(x, ...) <- value  
colData(x, ...)  
colData(x, ...) <- value  
#dim(x)  
#dimnames(x)  
#dimnames(x) <- value

## Quick colData access

## S4 method for signature 'SummarizedExperiment'

x$name

## 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, ...]] <- value

## Subsetting

## S4 method for signature 'SummarizedExperiment'

x[i, j, ..., drop=TRUE]

## S4 replacement method for signature 'SummarizedExperiment,ANY,ANY,SummarizedExperiment'

x[i, j] <- 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

x  
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 combined. For other accessors, ignored.

i, j For assay, assay<-, i is an integer or numeric scalar; see ‘Details’ for additional 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 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 ‘Details’.

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
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 doc-
umented in ?RangedSummarizedExperiment.

**Accessors**

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

```r
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]] <- value
to get or set the i th (default first) assay element. value must be a matrix of the same dimen-
sion 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.

```r
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

```r
x$name, x$name <- value Access or replace column name in x.

x[[i, ...]], x[[i, ...]] <- value Access or replace column i in x.

**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 on-disk realization of objects carrying delayed operations.
Examples

```r
nrows <- 200; ncols <- 6
counts <- matrix(runif(nrows * ncols, 1, 1e4), nrows)
colData <- DataFrame(Treatment=rep(c("ChIP", "Input"), 3),
                     row.names=LETTERS[1:6])
se0 <- SummarizedExperiment(assays=SimpleList(counts=counts),
                          colData=colData)
se0
dim(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)]
cmb1 <- cbind(se1, se2)
dim(cmb1)
dimnames(cmb1)

## rbind() combines objects with the same samples but different
## features of interest:
se1 <- se0
se2 <- se1[1:50,]ownames(se2) <- letters[1:nrow(se2)]
cmb2 <- rbind(se1, se2)
dim(cmb2)
dimnames(cmb2)

## ON-DISK REALIZATION
## ---------------------------------------------------------------------
setRealizationBackend("HDF5Array")
cmb3 <- realize(cmb2)
assay(cmb3, withDimnames=FALSE) # an HDF5Matrix object
```

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