Package ‘MultimodalExperiment’

April 4, 2024

Title     Integrative Bulk and Single-Cell Experiment Container
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Description MultimodalExperiment is an S4 class that integrates bulk and single-cell experiment data; it is optimally storage-efficient, and its methods are exceptionally fast. It effortlessly represents multimodal data of any nature and features normalized experiment, subject, sample, and cell annotations, which are related to underlying biological experiments through maps. Its coordination methods are opt-in and employ database-like join operations internally to deliver fast and flexible management of multimodal data.
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**annotation-methods**

**MultimodalExperiment Annotation Methods**

**Description**

joinAnnotations joins all annotations into an unnormalized `DataFrame` object.

**Usage**

```r
## S4 method for signature 'MultimodalExperiment'
joinAnnotations(x)
```

**Arguments**

- `x` a `MultimodalExperiment` object

**Value**

`joinAnnotations` returns a `DataFrame` object.

**See Also**

`browseVignettes("MultimodalExperiment")`

**Examples**

```r
ME <-
   MultimodalExperiment()

bulkExperiments(ME) <-
   ExperimentList(
         pbRNAseq = pbRNAseq
```
singleCellExperiments(ME) <-
  ExperimentList(
    scADTseq = scADTseq,
    scRNAseq = scRNAseq
  )

subjectMap(ME)[["subject"]]
  <-
  "SUBJECT-1"

sampleMap(ME)[["subject"]]
  <-
  "SUBJECT-1"

cellMap(ME)[["sample"]]
  <-
  "SAMPLE-1"

ME <-
  propagate(ME)

experimentData(ME)[["published"]]
  <-
  c(NA_character_, "2018-11-19", "2018-11-19") |> as.Date()

subjectData(ME)[["condition"]]
  <-
  as.character("healthy")

sampleData(ME)[["sampleType"]]
  <-
  as.character("peripheral blood mononuclear cells")

cellType <- function(x) {
  if (x[["CD4"]] > 0L) {
    return("T Cell")
  }

  if (x[["CD14"]] > 0L) {
    return("Monocyte")
  }

  if (x[["CD19"]] > 0L) {
    return("B Cell")
  }

  if (x[["CD56"]] > 0L) {
    return("NK Cell")
  }

  NA_character_
}

cellData(ME)[["cellType"]]
  <-
  experiment(ME, "scADTseq") |> apply(2L, cellType)
joinAnnotations(ME)

---

**MultimodalExperiment Coordination Methods**

**Description**

Propagate or harmonize indices of a MultimodalExperiment object.

**Usage**

```r
## S4 method for signature 'MultimodalExperiment'
propagate(x)
## S4 method for signature 'MultimodalExperiment'
harmonize(x)
```

**Arguments**

- `x`: a MultimodalExperiment object

**Details**

- **propagate** inserts experiment, subject, sample, and cell indices into all relevant tables by taking their union and adding missing indices.
- **harmonize** deletes experiment, subject, sample, and cell indices from all relevant tables by taking their intersection and removing extraneous indices.

**Value**

- **propagate** returns a MultimodalExperiment object.
- **harmonize** returns a MultimodalExperiment object.

**See Also**

- `browseVignettes("MultimodalExperiment")`

**Examples**

```r
ME <- MultimodalExperiment()
bulkExperiments(ME) <- ExperimentList(
  pbRNAseq = pbRNAseq
)
```
coordination-methods

```r
singleCellExperiments(ME) <- ExperimentList(
  scADTseq = scADTseq,
  scRNAseq = scRNAseq
)

subjectMap(ME)[["subject"]]<- "SUBJECT-1"

sampleMap(ME)[["subject"]]<- "SUBJECT-1"

cellMap(ME)[["sample"]]<- "SAMPLE-1"

ME <- propagate(ME)

experimentData(ME)[["published"]]<- c(NA_character_, "2018-11-19", "2018-11-19") |>
  as.Date()

subjectData(ME)[["condition"]]<- as.character("healthy")

sampleData(ME)[["sampleType"]]<- as.character("peripheral blood mononuclear cells")

cellType <- function(x) {
  if (x["CD4"] > 0L) {
    return("T Cell")
  }
  if (x["CD14"] > 0L) {
    return("Monocyte")
  }
  if (x["CD19"] > 0L) {
    return("B Cell")
  }
  if (x["CD56"] > 0L) {
    return("NK Cell")
  }
  NA_character_
}

cellData(ME)[["cellType"]]<- experiment(ME, "scADTseq") |>
  apply(2L, cellType)
```
isMonocyte <-
cellData(ME)[["cellType"]]%in% "Monocyte"

cellData(ME) <-
cellData(ME)[isMonocyte, , drop = FALSE]

harmonize(ME)

---

example-data  MultimodalExperiment Example Data

**Description**

Human peripheral blood mononuclear cells (PBMCs) from a single healthy donor were profiled by cellular indexing of transcriptomes and epitopes by sequencing (CITE-seq) to generate single-cell antibody-derived tag sequencing (scADTseq) and single-cell RNA sequencing (scRNAseq) data simultaneously; the scRNAseq data was summed into pseudo-bulk RNA sequencing (pbRNAseq) data. The dimensions of resulting matrices were reduced to conserve storage because these data are only used to demonstrate the functionality of the MultimodalExperiment class.

**Usage**

- pbRNAseq
- scADTseq
- scRNAseq

**Format**

- An object of class matrix (inherits from array) with 3000 rows and 1 columns.
- An object of class matrix (inherits from array) with 8 rows and 5000 columns.
- An object of class matrix (inherits from array) with 3000 rows and 5000 columns.

**Source**


**Examples**

- pbRNAseq[1:4, 1:1, drop = FALSE]
- scADTseq[1:4, 1:4, drop = FALSE]
- scRNAseq[1:4, 1:4, drop = FALSE]
**Description**

Extract or replace experiments of a `MultimodalExperiment` object by index, name, or type.

**Usage**

```r
## S4 method for signature 'MultimodalExperiment'
experiment(x, i)

## S4 replacement method for signature 'MultimodalExperiment'
experiment(x, i) <- value

## S4 method for signature 'MultimodalExperiment'
bulkExperiments(x)

## S4 replacement method for signature 'MultimodalExperiment'
bulkExperiments(x) <- value

## S4 method for signature 'MultimodalExperiment'
singleCellExperiments(x)

## S4 replacement method for signature 'MultimodalExperiment'
singleCellExperiments(x) <- value
```

**Arguments**

- `x` a `MultimodalExperiment` object
- `i` an integer or character index
- `value` a replacement value

**Details**

The term matrix-like objects refers to `matrix` objects or Bioconductor S4 objects that contain them (`SummarizedExperiment`, `SingleCellExperiment`, etc.) where rows represent features and columns represent observations.

**Value**

- `experiment` returns a matrix-like object.
- `bulkExperiments` returns an `ExperimentList` of matrix-like objects.
- `singleCellExperiments` returns an `ExperimentList` of matrix-like objects.
See Also

browseVignettes("MultimodalExperiment")

Examples

```
ME <- MultimodalExperiment()

bulkExperiments(ME) <- ExperimentList(
  pbRNAseq = pbRNAseq
)

singleCellExperiments(ME) <- ExperimentList(
  scADTseq = scADTseq,
  scRNAseq = scRNAseq
)

subjectMap(ME)[["subject"]] <- "SUBJECT-1"

sampleMap(ME)[["subject"]] <- "SUBJECT-1"

cellMap(ME)[["sample"]] <- "SAMPLE-1"

ME <- propagate(ME)

experimentData(ME)[["published"]] <-
  c(NA_character_, "2018-11-19", "2018-11-19") |> as.Date()

subjectData(ME)[["condition"]] <- as.character("healthy")

sampleData(ME)[["sampleType"]] <- as.character("peripheral blood mononuclear cells")

cellType <- function(x) {
  if (x["CD4"] > 0L) {
    return("T Cell")
  }

  if (x["CD14"] > 0L) {
    return("Monocyte")
  }

  if (x["CD19"] > 0L) {
    return("B Cell")
  }
}
```
if (x[['CD56']] > 0L) {
  return("NK Cell")
}

cellData(ME)[["cellType"]]<-
  experiment(ME, "scADTseq") |> apply(2L, cellType)

experiment(ME, 2L) <-
  experiment(ME, 2L)[1:4, 1:4]

experiment(ME, 2L)

experiment(ME, "scRNAseq") <-
  experiment(ME, "scRNAseq")[1:4, 1:4]

experiment(ME, "scRNAseq")

bulkExperiments(ME) <-
  bulkExperiments(ME)[1L]

bulkExperiments(ME)

singleCellExperiments(ME) <-
  singleCellExperiments(ME)[2L]

singleCellExperiments(ME)

---

### Description

`joinMaps` joins all maps into an unnormalized `DataFrame` object.

### Usage

```r
## S4 method for signature 'MultimodalExperiment'
joinMaps(x)
```

### Arguments

- `x` a `MultimodalExperiment` object
Value

joinMaps returns a DataFrame object.

See Also

browseVignettes("MultimodalExperiment")

Examples

```r
ME <- MultimodalExperiment()

bulkExperiments(ME) <- ExperimentList(
  pbRNAseq = pbRNAseq
)

singleCellExperiments(ME) <- ExperimentList(
  scADTseq = scADTseq,
  scRNAseq = scRNAseq
)

subjectMap(ME)[["subject"]]["SUBJECT-1"

sampleMap(ME)[["subject"]]["SUBJECT-1"

cellMap(ME)[["sample"]]["SAMPLE-1"

ME <- propagate(ME)

experimentData(ME)[["published"]]["2018-11-19", "2018-11-19"] |>
  as.Date()

subjectData(ME)[["condition"]]["healthy"

sampleData(ME)[["sampleType"]]["peripheral blood mononuclear cells"

cellType <- function(x) {
  if (x["CD4"] > 0L) {
    return("T Cell")
  }

  if (x["CD14"] > 0L) {
    return("Monocyte")
  }
```
if (x["CD19"] > 0L) {
    return("B Cell")
}
if (x["CD56"] > 0L) {
    return("NK Cell")
}

NA_character_

cellData(ME)["cellType"] <-
    experiment(ME, "scADTseq") |> apply(2L, cellType)

joinMaps(ME)
MultimodalExperiment

```r
  cell = character()
  ),
  experiments = ExperimentList(),
  metadata = list()
)
```

**Arguments**

- `experimentData` a `DataFrame` of experiment annotations with experiment indices as rownames
- `subjectData` a `DataFrame` of subject annotations with subject indices as rownames
- `sampleData` a `DataFrame` of sample annotations with sample indices as rownames
- `cellData` a `DataFrame` of cell annotations with cell indices as rownames
- `experimentMap` a `DataFrame` of type (bulk or single-cell) to experiment (index) mappings
- `subjectMap` a `DataFrame` of experiment (index) to subject (index) mappings
- `sampleMap` a `DataFrame` of subject (index) to sample (index) mappings
- `cellMap` a `DataFrame` of sample (index) to cell (index) mappings
- `experiments` an `ExperimentList` of matrix-like objects
- `metadata` a list of metadata objects

**Details**

The term matrix-like objects refers to `matrix` objects or Bioconductor S4 objects that contain them ( `SummarizedExperiment`, `SingleCellExperiment`, etc.) where rows represent features and columns represent observations.

**Value**

`MultimodalExperiment` returns a `MultimodalExperiment` object.

**See Also**

`browseVignettes("MultimodalExperiment")`

**Examples**

`MultimodalExperiment()`
MultimodalExperiment-class

MultimodalExperiment Class Definition

Description

MultimodalExperiment is an S4 class that integrates bulk and single-cell experiment data; it is optimally storage-efficient, and its methods are exceptionally fast. It effortlessly represents multimodal data of any nature and features normalized experiment, subject, sample, and cell annotations, which are related to underlying biological experiments through maps. Its coordination methods are opt-in and employ database-like join operations internally to deliver fast and flexible management of multimodal data.

Details

The term matrix-like objects refers to matrix objects or Bioconductor S4 objects that contain them (SummarizedExperiment, SingleCellExperiment, etc.) where rows represent features and columns represent observations.

Slots

experimentData a DataFrame of experiment annotations with experiment indices as rownames
subjectData a DataFrame of subject annotations with subject indices as rownames
sampleData a DataFrame of sample annotations with sample indices as rownames
cellData a DataFrame of cell annotations with cell indices as rownames
experimentMap a DataFrame of type (bulk or single-cell) to experiment (index) mappings
subjectMap a DataFrame of experiment (index) to subject (index) mappings
sampleMap a DataFrame of subject (index) to sample (index) mappings
cellMap a DataFrame of sample (index) to cell (index) mappings
experiments an ExperimentList of matrix-like objects
metadata a list of metadata objects

See Also

browseVignettes("MultimodalExperiment")
MultimodalExperiment Name Methods

Description

Extract or replace names of a MultimodalExperiment object.

Usage

```r
## S4 method for signature 'MultimodalExperiment'
names(x)

## S4 replacement method for signature 'MultimodalExperiment'
names(x) <- value

## S4 method for signature 'MultimodalExperiment'
rownames(x)

## S4 replacement method for signature 'MultimodalExperiment'
rownames(x) <- value

## S4 method for signature 'MultimodalExperiment'
colnames(x)

## S4 replacement method for signature 'MultimodalExperiment,ANY'
colnames(x) <- value

## S4 method for signature 'MultimodalExperiment'
dimnames(x)

## S4 replacement method for signature 'MultimodalExperiment,ANY'
dimnames(x) <- value

## S4 method for signature 'MultimodalExperiment'
experimentNames(x)

## S4 replacement method for signature 'MultimodalExperiment'
experimentNames(x) <- value
```

Arguments

- `x` a MultimodalExperiment object
- `value` a replacement value

Value

names returns a CharacterList object.
rownames returns a CharacterList object.
colnames returns a CharacterList object.
dimnames returns a list object.
experimentNames returns a character vector.

See Also

browseVignettes("MultimodalExperiment")

Examples

ME <-
  MultimodalExperiment()

bulkExperiments(ME) <-
  ExperimentList(
    pbRNAseq = pbRNAseq
  )

singleCellExperiments(ME) <-
  ExperimentList(
    scADTseq = scADTseq,
    scRNAseq = scRNAseq
  )

subjectMap(ME)[["subject"]]<-
  "SUBJECT-1"

sampleMap(ME)[["subject"]]<-
  "SUBJECT-1"

cellMap(ME)[["sample"]]<-
  "SAMPLE-1"

ME <-
  propagate(ME)

experimentData(ME)[["published"]]<-
  c(NA_character_, "2018-11-19", "2018-11-19") |> as.Date()

subjectData(ME)[["condition"]]<-
  as.character("healthy")

sampleData(ME)[["sampleType"]]<-
  as.character("peripheral blood mononuclear cells")

cellType <- function(x) {
  if (x["CD4"] > 0L) {
    return("T Cell")
  }
}
if (x["CD14"] > 0L) {
  return("Monocyte")
}
if (x["CD19"] > 0L) {
  return("B Cell")
}
if (x["CD56"] > 0L) {
  return("NK Cell")
}
NA_character_

cellData(ME)[["cellType"]]
  <-
  experiment(ME, "scADTseq") |> apply(2L, cellType)

names(ME) <-
  names(ME) |> tolower()

rownames(ME) <-
  rownames(ME) |> toupper()

colnames(ME) <-
  colnames(ME) |> tolower()

dimnames(ME)[[2L]] <-
  dimnames(ME)[[2L]] |> toupper()

dimnames(ME)[[2L]]
experimentNames(ME) <-
  experimentNames(ME) |> gsub(pattern = "seq", replacement = "-seq")
experimentNames(ME)
Objects exported from other packages

Description
These objects are imported from other packages. Follow the links below to see their documentation.

MultiAssayExperiment  ExperimentList

show-method  MultimodalExperiment Show Method

Description
Display details about a MultimodalExperiment object.

Usage
```r
## S4 method for signature 'MultimodalExperiment'
show(object)
```

Arguments
- **object**: a MultimodalExperiment object

Value
- `show` returns NULL invisibly.

See Also
- `browseVignettes("MultimodalExperiment")`

Examples
```r
ME <- MultimodalExperiment()

bulkExperiments(ME) <- ExperimentList(
  pbRNAseq = pbRNAseq
)

singleCellExperiments(ME) <- ExperimentList(
  scADTseq = scADTseq,
  scRNAseq = scRNAseq
)```
subjectMap(ME)[["subject"]]
  <-
  "SUBJECT-1"

sampleMap(ME)[["subject"]]
  <-
  "SUBJECT-1"

cellMap(ME)[["sample"]]
  <-
  "SAMPLE-1"

ME <-
  propagate(ME)

experimentData(ME)[["published"]]
  <-
  c(NA_character_, "2018-11-19", "2018-11-19") |> as.Date()

subjectData(ME)[["condition"]]
  <-
  as.character("healthy")

sampleData(ME)[["sampleType"]]
  <-
  as.character("peripheral blood mononuclear cells")

cellType <- function(x) {
  if (x["CD4"] > 0L) {
    return("T Cell")
  }
  if (x["CD14"] > 0L) {
    return("Monocyte")
  }
  if (x["CD19"] > 0L) {
    return("B Cell")
  }
  if (x["CD56"] > 0L) {
    return("NK Cell")
  }
  NA_character_
}

cellData(ME)[["cellType"]]
  <-
  experiment(ME, "scADTseq") |> apply(2L, cellType)

show(ME)
slot-methods

MultimodalExperiment Slot Methods

Description

Extract or replace slots of a MultimodalExperiment object.

Usage

```r
## S4 method for signature 'MultimodalExperiment'
experimentData(object)

## S4 replacement method for signature 'MultimodalExperiment'
experimentData(object) <- value

## S4 method for signature 'MultimodalExperiment'
subjectData(object)

## S4 replacement method for signature 'MultimodalExperiment'
subjectData(object) <- value

## S4 method for signature 'MultimodalExperiment'
sampleData(object)

## S4 replacement method for signature 'MultimodalExperiment'
sampleData(object) <- value

## S4 method for signature 'MultimodalExperiment'
cellData(object)

## S4 replacement method for signature 'MultimodalExperiment'
cellData(object) <- value

## S4 method for signature 'MultimodalExperiment'
experimentMap(object)

## S4 replacement method for signature 'MultimodalExperiment'
experimentMap(object) <- value

## S4 method for signature 'MultimodalExperiment'
subjectMap(object)

## S4 replacement method for signature 'MultimodalExperiment'
subjectMap(object) <- value

## S4 method for signature 'MultimodalExperiment'
sampleMap(object)
```
## S4 replacement method for signature 'MultimodalExperiment'
```r
sampleMap(object) <- value
```

## S4 method for signature 'MultimodalExperiment'
```r
cellMap(object)
```

## S4 replacement method for signature 'MultimodalExperiment'
```r
object <- value
```

## S4 method for signature 'MultimodalExperiment'
```r
experiments(object)
```

## S4 replacement method for signature 'MultimodalExperiment'
```r
experiments(object) <- value
```

### Arguments

- `object`: a `MultimodalExperiment` object
- `value`: a replacement value

### Value

Extract methods return the value of the slot.

### See Also

`browseVignettes("MultimodalExperiment")`

### Examples

```r
ME <- MultimodalExperiment()
bulkExperiments(ME) <- ExperimentList(
  pbRNAseq = pbRNAseq
)
singleCellExperiments(ME) <- ExperimentList(
  scADTseq = scADTseq,
  scRNAseq = scRNAseq
)
subjectMap(ME)[["subject"]] <- "SUBJECT-1"
sampleMap(ME)[["subject"]] <- "SUBJECT-1"
```
cellMap(ME)["sample"] <-
  "SAMPLE-1"

ME <-
  propagate(ME)

experimentData(ME)["published"] <-
  c(NA_character_, "2018-11-19", "2018-11-19") |> as.Date()

subjectData(ME)["condition"] <-
  as.character("healthy")

sampleData(ME)["sampleType"] <-
  as.character("peripheral blood mononuclear cells")

cellType <- function(x) {
  if (x["CD4"] > 0L) {
    return("T Cell")
  }
  if (x["CD14"] > 0L) {
    return("Monocyte")
  }
  if (x["CD19"] > 0L) {
    return("B Cell")
  }
  if (x["CD56"] > 0L) {
    return("NK Cell")
  }
  NA_character_
}

cellData(ME)["cellType"] <-
  experiment(ME, "scADTseq") |> apply(2L, cellType)

experimentData(ME)

subjectData(ME)

sampleData(ME)

cellData(ME)

experimentMap(ME)

subjectMap(ME)

sampleMap(ME)
subset-methods

MultimodalExperiment Subset Methods

Description

Extract or replace parts of a MultimodalExperiment object.

Usage

```r
## S4 method for signature 'MultimodalExperiment,ANY,ANY,ANY'
x[i, j, ..., drop = FALSE]
## S4 replacement method for signature 'MultimodalExperiment,ANY,ANY,ANY'
x[i, j] <- value
```

Arguments

- **x**: a MultimodalExperiment object
- **i**: a list, List, LogicalList, IntegerList, or CharacterList of elements to extract or replace
- **j**: a list, List, LogicalList, IntegerList, or CharacterList of elements to extract or replace
- **...**: ignored, required by generic
- **drop**: ignored, required by generic
- **value**: a replacement value

Value

[ returns a MultimodalExperiment object.

See Also

browseVignettes("MultimodalExperiment")
Examples

```r
ME <- MultimodalExperiment()

bulkExperiments(ME) <-
  ExperimentList(
    pbRNAseq = pbRNAseq
  )

singleCellExperiments(ME) <-
  ExperimentList(
    scADTseq = scADTseq,
    scRNAseq = scRNAseq
  )

subjectMap(ME)["subject"] <-
  "SUBJECT-1"

sampleMap(ME)["subject"] <-
  "SUBJECT-1"

cellMap(ME)["sample"] <-
  "SAMPLE-1"

ME <-
  propagate(ME)

experimentData(ME)["published"] <-
  c(NA_character_, "2018-11-19", "2018-11-19") |> as.Date()

subjectData(ME)["condition"] <-
  as.character("healthy")

sampleData(ME)["sampleType"] <-
  as.character("peripheral blood mononuclear cells")

cellType <- function(x) {
  if (x["CD4"] > 0L) {
    return("T Cell")
  }
  if (x["CD14"] > 0L) {
    return("Monocyte")
  }
  if (x["CD19"] > 0L) {
    return("B Cell")
  }
  if (x["CD56"] > 0L) {
    return("NK Cell")
  }
}
```
NA_character_

```r

cellData(ME)["cellType"] <-
  experiment(ME, "scADTseq") |>
  apply(2L, cellType)

i <-
  rownames(ME) |>  
  endoapply(sample, 4L)

j <-
  colnames(ME) |>  
  endoapply(sample, 1L)

ME[i, j] <-
  0L

experiment(ME[i, j], "pbRNAseq")
experiment(ME[i, j], "scADTseq")
experiment(ME[i, j], "scRNAseq")
```
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