Package ‘MultiDataSet’

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Type Package

Title Implementation of the BRGE’s (Bioinformatic Research Group in Epidemiology from Center for Research in Environmental Epidemiology) MultiDataSet and MethylationSet

Version 1.2.0

Description Implementation of the BRGE’s (Bioinformatic Research Group in Epidemiology from Center for Research in Environmental Epidemiology) MultiDataSet and MethylationSet. MultiDataSet is designed for integrating multi omics data sets and MethylationSet to contain normalized methylation data. These package contains base classes for MEAL and rexposome packages.

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LazyData TRUE

biocViews Software, DataRepresentation

Depends R (>= 3.3), Biobase

Imports BiocGenerics, GenomicRanges, IRanges, minfi, S4Vectors, SummarizedExperiment, methods, IlluminaHumanMethylation450kanno.ilmn12.hg19, utils

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add_eset

Method to add an eSet to MultiDataSet.

Description
This method adds or overwrites a slot of a MultiDataSet with the content of the given eSet.

Usage
add_eset(object, set, dataset.type, dataset.name = NULL, warnings = TRUE, overwrite = FALSE, GRanges)

Arguments
object MultiDataSet that will be filled.
set Object derived from eSet to be used to fill the slot.
dataset.type Character with the type of data of the omic set (e.g. expression, methylation...)
dataset.name Character with the specific name for this set (NULL by default). It is useful when there are several sets of the same type (e.g. multiple expression assays)
warnings Logical to indicate if warnings will be displayed.
overwrite Logical to indicate if the set stored in the slot will be overwritten.
GRanges GenomicRanges to be included in rowRanges slot.

Value
A new MultiDataSet with a slot filled.

See Also
add_methy, add_genexp, add_rnaseq, add_snps

Examples
multi <- createMultiDataSet()
eset <- new("ExpressionSet", exprs = matrix(runif(10), 5))
multi <- add_eset(multi, eset, "exampledata", GRanges = NA)
add_genexp

Method to add an expression microarray dataset to MultiDataSet.

Description

This method adds or overwrites the slot "expression" of a MultiDataSet with the content of the given ExpressionSet. The fData of the ExpressionSet must contain the columns chromosome, start and end.

Usage

add_genexp(object, gexpSet, ...)

Arguments

- object: MultiDataSet that will be filled.
- gexpSet: ExpressionSet to be used to fill the slot.
- ...: Arguments to be passed to add_eset.

Value

A new MultiDataSet with the slot "expression" filled.

Examples

```r
multi <- createMultiDataSet()
eset <- new("ExpressionSet", exprs = matrix(runif(4), 2))
fData(eset) <- data.frame(chromosome = c("chr1", "chr2"), start = c(12414, 1234321),
                         end = c(121241, 124124114), stringsAsFactors = FALSE)
multi <- add_genexp(multi, eset)
```

add_methy

Method to add a slot of methylation to MultiDataSet.

Description

This method adds or overwrites the slot "methylation" of a MultiDataSet with the content of the given MethylationSet or RatioSet. The fData of the input object must contain the columns chromosome and position.

Usage

add_methy(object, methySet, ...)

Arguments

- object: MultiDataSet that will be filled.
- methySet: MethylationSet or RatioSet to be used to fill the slot.
- ...: Further arguments to be passed to add_eset.
**Value**

A new MultiDataSet with the slot "methylation" filled.

**Examples**

```r
if (require(MEALData)){
  multi <- createMultiDataSet()
  betavals <- betavals[1:100, ]  ## To speed up the example, the beta values are reduced
  methy <- prepareMethylationSet(betavals, pheno)
  multi <- add_methy(multi, methy)
}
```

---

**add_rnaseq**  
Method to add an expression RNA seq dataset to MultiDataSet.

**Description**

This method adds or overwrites the slot "rnaseq" of an MultiDataSet with the content of the given ExpressionSet. The fData of the ExpressionSet must contain the columns chromosome, start and end.

**Usage**

```r
add_rnaseq(object, rnaSet, ...)
```

**Arguments**

- **object**  
  MultiDataSet that will be filled.
- **rnaSet**  
  ExpressionSet to be used to fill the slot.
- **...**  
  Arguments to be passed to add_eset.

**Value**

A new MultiDataSet with the slot "rnaseq" filled.

**Examples**

```r
multi <- createMultiDataSet()
eset <- new("ExpressionSet", exprs = matrix(runif(4), 2))
fData(eset) <- data.frame(chromosome = c("chr1", "chr2"), start = c(12414, 1234321),
end = c(121241, 12122414), stringsAsFactors = FALSE)
multi <- add_genexp(multi, eset)
```
Method to add a RangedSummarizedExperiment to MultiDataSet.

Description

This method adds or overwrites a slot of a MultiDataSet with the content of the given RangedSummarizedExperiment.

Usage

add_rse(object, set, dataset.type, dataset.name = NULL, warnings = TRUE, overwrite = FALSE)

Arguments

object MultiDataSet that will be filled.
set Object derived from RangedSummarizedExperiment to be used to fill the slot.
dataset.type Character with the type of data of the omic set (e.g. expression, methylation...)
dataset.name Character with the specific name for this set (NULL by default). It is useful when there are several sets of the same type (e.g. multiple expression assays)
warnings Logical to indicate if warnings will be displayed.
overwrite Logical to indicate if the set stored in the slot will be overwritten.

Value

A new MultiDataSet with a slot filled.

Examples

if (require(GenomicRanges) & require(SummarizedExperiment)){
  multi <- createMultiDataSet()
  counts <- matrix(runif(200 * 6, 1, 1e4), 200)
  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], id = LETTERS[1:6])
  names(rowRanges) <- 1:200
  rse <- SummarizedExperiment(assays=SimpleList(counts=counts),
    rowRanges=rowRanges, colData=colData)
  multi <- add_rse(multi, rse, "rseEx")
}
add_snps

Method to add a slot of SNPs to MultiDataSet.

Description

This method adds or overwrites the slot "snps" of an MultiDataSet with the content of the given SnpSet. The fData of the SnpSet must contain the columns chromosome and position.

Usage

```r
add_snps(object, snpSet, ...)  
```

Arguments

- `object` MultiDataSet that will be filled.
- `snpSet` SnpSet to be used to fill the slot.
- `...` Arguments to be passed to add_eset.

Value

A new MultiDataSet with the slot "snps" filled.

Examples

```r
multi <- createMultiDataSet()
geno <- matrix(c(3,1,2,1), ncol = 2)
colnames(geno) <- c("VAL0156", "VAL0372")
rownames(geno) <- c("rs3115860", "SNP1-1628854")
map <- AnnotatedDataFrame(data.frame(chromosome = c("chr1", "chr2"), position = c(12414, 1234321), stringsAsFactors = FALSE))
rownames(map) <- rownames(geno)
snpSet <- new("SnpSet", call = geno, featureData = map)
pheno <- data.frame(id = c("VAL0156", "VAL0372"))
rownames(pheno) <- c("VAL0156", "VAL0372")
pData(snpSet) <- pheno
multi <- add_snps(multi, snpSet)
```

checkProbes

Filter MethylationSet probes

Description

This function selects probes present in the annotation matrix. Probes without annotation and annotation values without beta values are discarded.

Usage

```r
checkProbes(object)
```
checkSamples

Arguments

object     MethylationSet

Value

MethylationSet containing the common samples.

Examples

if (require(MEALData)){
  betavals <- betavals[1:100, ]  ## To speed up the example, the beta values are reduced
  methy <- prepareMethylationSet(betavals, pheno)
  checkProbes(methy)
}

Description

This function removes samples that have beta values but no phenotypes and vice versa. If snps object is present, only samples present in the three set are retained.

Usage

checkSamples(object)

Arguments

object     MethylationSet

Value

MethylationSet containing the common samples.

Examples

if (require(MEALData)){
  betavals <- betavals[1:100, ]  ## To speed up the example, the beta values are reduced
  methy <- prepareMethylationSet(betavals, pheno)
  checkSamples(methy)
}
**chrNumToChar**

*Convert chr numbers to chr strings*

**Description**

Given a vector of number representing the chromosomes, convert them to string (e.g 1 to chr1). 23 is considered chrX, 24 is chrY, 25 is chrXY (probes shared between chromosomes X and Y) and 26 is chrMT.

**Usage**

```r
chrNumToChar(vector)
```

**Arguments**

- `vector` The vector with the chromosome numbers

**Value**

A vector with the chromosomes in string format.

**Examples**

```r
chromosomes <- c(1, 3, 4, 23, 15)
stringsChrs <- chrNumToChar(chromosomes)
stringsChrs
```

---

**commonIds**

*Get the name of the ids common to all datasets*

**Description**

Get the name of the ids common to all datasets.

**Usage**

```r
commonIds(object)
```

**Arguments**

- `object` MultiDataSet that will be filtered.

**Value**

Character vector with the common ids.
commonSamples

Examples

multi <- createMultiDataSet()
eset <- new("ExpressionSet", exprs = matrix(runif(9), ncol = 3))
fData(eset) <- data.frame(chromosome = c("chr1", "chr1", "chr1"),
                        start = c(1, 5, 10), end = c(4, 6, 14),
                        stringsAsFactors = FALSE)
sampleNames(eset) <- c("S1", "S2", "S3")
pData(eset) <- data.frame(id = c("S1", "S2", "S3"))
rownames(pData(eset)) <- c("S1", "S2", "S3")
multi <- add_genexp(multi, eset, dataset.name = "g1")
eset <- new("ExpressionSet", exprs = matrix(runif(8), ncol = 2))
fData(eset) <- data.frame(chromosome = c("chr1", "chr1", "chr1", "chr1"),
                        start = c(1, 14, 25, 104), end = c(11, 16, 28, 115),
                        stringsAsFactors = FALSE)
sampleNames(eset) <- c("S1", "G2")
pData(eset) <- data.frame(id = c("S1", "G2"))
rownames(pData(eset)) <- c("S1", "G2")
multi <- add_genexp(multi, eset, dataset.name = "g2")
commonIds(multi)

commonSamples
Method to select samples that are present in all datasets.

Description
This method subsets the datasets to only contain the samples that are in all datasets.

Usage
commonSamples(object)

Arguments
object MultiDataSet that will be filtered.

Value
A new MultiDataSet with only the common samples.

Examples

multi <- createMultiDataSet()
eset <- new("ExpressionSet", exprs = matrix(runif(9), ncol = 3))
fData(eset) <- data.frame(chromosome = c("chr1", "chr1", "chr1"),
                        start = c(1, 5, 10), end = c(4, 6, 14),
                        stringsAsFactors = FALSE)
sampleNames(eset) <- c("S1", "S2", "S3")
pData(eset) <- data.frame(id = c("S1", "S2", "S3"))
rownames(pData(eset)) <- c("S1", "S2", "S3")
multi <- add_genexp(multi, eset, dataset.name = "g1")
eset <- new("ExpressionSet", exprs = matrix(runif(8), ncol = 2))
fData(eset) <- data.frame(chromosome = c("chr1", "chr1", "chr1", "chr1"),
    start = c(1, 14, 25, 104),
    end = c(11, 16, 28, 115),
    stringsAsFactors = FALSE)
sampleNames(eset) <- c("S1", "G2")
pData(eset) <- data.frame(id = c("S1", "G2"))
rownames(pData(eset)) <- c("S1", "G2")

multi <- add_genexp(multi, eset, dataset.name="g2")
commonSamples(multi)

getMs

Transforms beta values to M-values

Description
Given a MethylationSet or a AnalysisResults returns the matrix of M values using a logit2 transformation. Betas equal to 0 will be transformed to threshold and betas equal to 1, to 1 - threshold.

Usage
getMs(object, threshold = 1e-04)

Arguments
object MethylationSet or AnalysisResults
threshold Numeric with the threshold to avoid 0s and 1s.

Value
Matrix with the M values.

Examples
if (require(minfiData)){
    set <- prepareMethylationSet(MsetEx[1:100, ], pData(MsetEx))
    mvalues <- getMs(set)
    head(mvalues)
}

MethylationSet

MethylationSet instances

Description
Container with the data needed to perform methylation analysis. MethylationSet inherits from eSet and contains meth matrix as assay data member.
Usage

methylationSet(betas, phenotypes, annotationDataFrame, annoString = "custom")

## S4 method for signature 'MethylationSet'
betas(object)

## S4 method for signature 'MethylationSet'
getMs(object, threshold = 1e-04)

## S4 method for signature 'MethylationSet'
checkProbes(object)

## S4 method for signature 'MethylationSet'
checkSamples(object)

Arguments

betas Matrix of beta values
phenotypes Data.frame or AnnotatedDataFrame with the phenotypes
annotationDataFrame Data.frame or AnnotatedDataFrame with the phenotypes with the annotation of the methylation sites. A column with the chromosomes named chr and a column with the positions names pos are required.
annoString Character with the name of the annotation used.
object MethylationSet
threshold Numeric with the threshold to avoid 0s and 1s.

Details

FeatureData, which contains annotation data, is required to perform any of the analysis.

Value

MethylationSet

Methods (by generic)

• betas: Get beta matrix
• getMs: Get Ms values
• checkProbes: Filter probes with annotation
• checkSamples: Modify a MethylationSet to only contain common samples

Slots

assayData Contains matrices with equal dimensions, and with column number equal to nrow(phenData). assayData must contain a matrix meth with rows representing features (e.g., methylation probes sets) and columns representing samples.

phenodata See eSet

annotation See eSet

featureData See eSet. fData should contain at least chromosome and positions columns.
MultiDataSet-class

Examples

showClass("MethylationSet")

MultiDataSet: Implementation of the BRGE's basic classes

Description

Implementation of the BRGE's (Bioinformatic Research Group in Epidemiology from Center for Research in Environmental Epidemiology) MultiDataSet and MethylationSet. MultiDataSet is designed for integrating multi-omics data sets and MethylationSet to contain normalized methylation data. MultiDataSet for integrating multi-omics data sets

See Also

MultiDataSet

MultiDataSet-class

MultiDataSet instances

Description

The class MultiDataSet is a superior class to store multiple datasets in form of triplets (assayData, phenoData, featureData). The datasets must be eSet or SummarizedExperiment.

Usage

```r
## S4 method for signature 'MultiDataSet,eSet'
add_eset(object, set, dataset.type, 
    dataset.name = NULL, warnings = TRUE, overwrite = FALSE, GRanges)

## S4 method for signature 'MultiDataSet,ExpressionSet'
add_genexp(object, gexpSet, ...)

## S4 method for signature 'MultiDataSet,ExpressionSet'
add_rnaseq(object, rnaSet, ...)

## S4 method for signature 'MultiDataSet,MethylationSet'
add_methy(object, methySet, ...)

## S4 method for signature 'MultiDataSet,RatioSet'
add_methy(object, methySet, ...)

## S4 method for signature 'MultiDataSet,RangedSummarizedExperiment'
add_rse(object, set, 
    dataset.type, dataset.name = NULL, warnings = TRUE, overwrite = FALSE)

## S4 method for signature 'MultiDataSet,SnpSet'
add_snps(object, snpSet, ...)
```
## S4 method for signature 'MultiDataSet'
as.list(x)

## S4 method for signature 'MultiDataSet'
assayData(object)

## S4 method for signature 'MultiDataSet'
commonIds(object)

## S4 method for signature 'MultiDataSet'
commonSamples(object)

createMultiDataSet()

## S4 method for signature 'MultiDataSet'
fData(object)

## S4 method for signature 'MultiDataSet'
w_iclusterplus(object, commonSamples = TRUE, ...)

## S4 method for signature 'MultiDataSet'
length(x)

## S4 method for signature 'MultiDataSet'
rowRanges(x)

## S4 method for signature 'MultiDataSet'
x[[i]]

## S4 method for signature 'MultiDataSet'
x[i, j, k, ..., drop = FALSE]

## S4 method for signature 'MultiDataSet'
sampleNames(object)

## S4 method for signature 'MultiDataSet'
pData(object)

## S4 method for signature 'MultiDataSet'
rowRanges(x)

## S4 method for signature 'MultiDataSet'
subset(x, feat, phe, warnings = TRUE, keep = TRUE)
**MultiDataSet-class**

**Arguments**

- **object**: `MultiDataSet`
- **set**: Object derived from `eSet` to be used to fill the slot.
- **dataset.type**: Character with the type of data of the omic set (e.g. expression, methylation...)
- **dataset.name**: Character with the specific name for this set (NULL by default). It is useful when there
- **warnings**: Logical to indicate if warnings will be displayed.
- **overwrite**: Logical to indicate if the set stored in the slot will be overwritten.
- **GRanges**: GenomicRanges to be included in rowRanges slot.
- **gexpSet**: ExpressionSet to be used to fill the slot.
- **...**: Further arguments passed to `add_eset`.
- **rnaSet**: ExpressionSet to be used to fill the slot.
- **methySet**: MethylationSet to be used to fill the slot.
- **snpSet**: SnpSet to be used to fill the slot.
- **x**: `MultiDataSet`
- **commonSamples**: Logical to indicate if common samples are selected
- **i**: Character corresponding to selected sample names. They should match the id column of phenoData.
- **j**: Character with the name of the selected tables.
- **k**: GenomicRange used to filter the features.
- **drop**: If TRUE, sets with no samples or features will be discarded
- **feat**: Logical expression indicating features to keep
- **phe**: Logical expression indicating the phenotype of the samples to keep
- **keep**: If FALSE, sets where the expression cannot be evaluated will be discarded.

**Details**

The names of the three lists (assayData, phenoData and featureData) must be the same.

**Value**

`MultiDataSet`

**Methods (by generic)**

- **add_eset**: Method to add an `eSet` to `MultiDataSet`.
- **add_genexp**: Method to add a slot of expression to `MultiDataSet`.
- **add_rnaseq**: Method to add a slot of (RNASeq) expression to `MultiDataSet`.
- **add_methy**: Method to add a slot of methylation to `MultiDataSet`.
- **add_rse**: Method to add a `RangedSummarizedExperiment` to `MultiDataSet`.
- **add_snps**: Method to add a slot of SNPs to `MultiDataSet`.
- **as.list**: Returns a list with the first matrix of each dataset.
- **assayData**: Retrieve all assay data blocks.
prepareMethylationSet

- commonIds: Get the name of the ids common to all datasets
- commonSamples: Get a MultiDataSet only with the samples present in all the tables
- pData: Retrieve information on features.
- w_iclusterplus: Apply iClusterPlus clustering method to a MultiDataSet object
- length: Returns the number of sets into the object.
- w_mcia: Apply mcia integration method to a MultiDataSet object
- names: Get the names of the slots.
- rowRangesElements: Get the name of the datasets that have rowRanges
- sampleNames: Get sample names
- pData: Retrieve information on experimental phenotypes.
- rowRanges: Retrieve information on feature ranges.
- ::: Get a set from a slot
- :: Subset a MultiDataSet
- subset: Filter a subset using feature ids or phenotypes

Slots

- assayData List of assayData elements.
- phenoData List of AnnotatedDataFrame containing the phenoData of each assayData.
- featureData List of AnnotatedDataFrame containing the featureData of each assayData.
- rowRanges List of GenomicRanges containing the rowRanges of each assayData.
- return_method List of functions used to create the original object.

See Also

add_eset, add_rse

Examples

createMultiDataSet()

prepareMethylationSet  Generating a MethylationSet

Description

This function creates a MethylationSet using from a matrix of beta values and a data.frame of phenotypes.

Usage

prepareMethylationSet(matrix, phenotypes,
  annotation = "illuminaHumanMethylation450kanno.ilmn12.hg19",
  chromosome = "chr", position = "pos", genes = "UCSC_RefGene_Name",
  group = "UCSC_RefGene_Group", filterNA_threshold = 0.05,
  verbose = FALSE)
prepareMethylationSet

Arguments

- **matrix**: Data.frame or a matrix with samples on the columns and cpgs on the rows. A minfi object can be used to.
- **phenotypes**: Data.frame or vector with the phenotypic features of the samples. Samples will be in the rows and variables in the columns. If matrix is a minfi object, phenotypes can be taken from it.
- **annotation**: Character with the name of the annotation package or data.frame or AnnotationDataFrame with the annotation.
- **chromosome**: Character with the column containing chromosome name in the annotation data.
- **position**: Character with the column containing position coordinate in the annotation data.
- **genes**: Character with the column containing gene names related to the methylation site in the annotation data. (Optional)
- **group**: Character with the column containing the position of the probe related to the gene named in gene column. (Optional)
- **filterNA_threshold**: Numeric with the maximum percentage of NA allowed for each of the probes. If 1, there will be no filtering, if 0 all probes containing at least a NA will be filtered.
- **verbose**: Logical value. If TRUE, it writes out some messages indicating progress. If FALSE nothing should be printed.

Details

prepareMethylationSet is a useful wrapper to create MethylationSet. Right now, prepareMethylationSet supports two entry points: a minfi object and a matrix of betas.

Phenotypes are compulsory and can be supplied as data.frame or AnnotatedDataFrame.

By default, annotation is taken from minfi package and IlluminaHumanMethylation450kanno.ilmn12.hg19 package is used, being the default arguments adapted to use this annotation. To use this annotation, IlluminaHumanMethylation450kanno.ilmn12.hg19 must be installed and methylation sites must be named like in Illumina 450k chip. Use of this annotation ensures correct results in all the analysis.

If custom annotation is desired, there are two compulsory features: chromosomes and positions. Chromosomes should be supplied in the character form (e.g. chr1). Two additional features will be used during the presentation of results but not during the analyses: genes and group. Genes are the gene names of the genes around the cpg site and group defines the groups of the genes. Both columns will appear in the results but they are not used through the workflow. It should be noticed that BlockFinder only supports minfi annotation, so it is not advised to be used with custom annotation.

Value

MethylationSet with phenotypes and annotation.

Examples

```r
if (require(minfiData)){
  betas <- getBeta(MsetEx)[1:1000, ]
  pheno <- pData(MsetEx)
  set <- prepareMethylationSet(betas, pheno)
}
```
**rowRangesElements**

Get the name of the datasets that have rowRanges

**Description**

Get the name of the datasets that have rowRanges

**Usage**

```r
rowRangesElements(object)
```

**Arguments**

- **object** MultiDataSet

**Value**

Character vector with the slots that have rowRanges.

**Examples**

```r
multi <- createMultiDataSet()
eset <- new("ExpressionSet", exprs = matrix(runif(10), 5))
eset2 <- new("ExpressionSet", exprs = matrix(runif(8), ncol = 2))
fData(eset2) <- data.frame(chromosome = c("chr1", "chr1", "chr1", "chr1"),
                         start = c(1, 14, 25, 104),
                         end = c(11, 16, 28, 115),
                         stringsAsFactors = FALSE)
multi <- add_eset(multi, eset, "exampledata", GRanges = NA)
multi <- add_genexp(multi, eset2)
rowRangesElements(multi)
```

---

**w_iclusterplus**

Apply iClusterPlus clustering method to a MultiDataSet object

**Description**

Method iClusterPlus is applied on a MultiDataSet object after getting the common samples along all the contained datasets.

**Usage**

```r
w_iclusterplus(object, commonSamples = TRUE, ...)
```

**Arguments**

- **object** MultiDataSet
- **commonSamples** Logical to indicate if common samples are selected
- **...** Arguments passed to function iClusterPlus
Value

A list of results from iClusterPlus

Note

Argument type for iClusterPlus is filled within the method.

---

w_mcia  

Apply mcia integration method to a MultiDataSet object

---

Description

Method mcia is applied on a MultiDataSet object after getting the common samples along all the contained datasets.

Usage

w_mcia(object, ...)

Arguments

<table>
<thead>
<tr>
<th>object</th>
<th>MultiDataSet</th>
</tr>
</thead>
<tbody>
<tr>
<td>...</td>
<td>Arguments passed to function mcia</td>
</tr>
</tbody>
</table>

Value

A list of results from mcia
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