

Package ‘GraphExperiment’

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Title S4 Class for Quantitative Data and Associated Networks

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Description GraphExperiment provides users and developers with an S4 class that extends `SingleCellExperiment` by offering infrastructure to store and retrieve networks (`igraph` objects) representing how assay features and/or observations are associated with each other. The class was designed to store networks inferred from high-dimensional quantitative data, with feature-feature networks including gene coexpression networks (GCNs), gene regulatory networks (GRNs), and co-abundance networks (from proteomics and metabolomics), and observation-observation network including cell-cell distances, species-species relationships, and sample-sample similarities.

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URL <https://github.com/almeidasilvaf/GraphExperiment>

BugReports <https://support.bioconductor.org/tag/GraphExperiment>

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GraphExperiment-class GraphExperiment *S4 class*

Description

The GraphExperiment class was designed to represent rectangular, quantitative data (e.g., from transcriptomics, proteomics, metabolomics) along with graphs showing how features (e.g., genes, proteins, compounds) and observations (e.g., samples, cells, species, spots) interact with each other. It extends SingleCellExperiment by providing users with additional slots where row/column graphs can be stored.

Usage

```
GraphExperiment(..., rowGraphs = list(), colGraphs = list())
```

Arguments

...	Arguments passed to the SingleCellExperiment constructor function.
rowGraphs	A list of igraph objects with one or multiple graphs representing how features relate to each other. Node names (i.e., $V(\text{graph})\$name$) must match rownames of assays.
colGraphs	A list of igraph objects with one or multiple graphs representing how observations relate to each other. Node names (i.e., $V(\text{graph})\$name$) must match colnames of assays.

Details

Like `SingleCellExperiment`, the `GraphExperiment` S4 class stores quantitative data with associated metadata (i.e., `rowData` and `colData`) along with embeddings from dimensionality reduction techniques. However, it provides users with additional containers for `igraph` objects containing graphs describing how features and/or observations interact with each other. Graphs for features are stored in a `rowGraphs` slot, and graphs for observations are stored in a `colGraphs` slot. Both slots can hold one or multiple `igraph` objects with some sort of network representation of the features in `rownames` or observations in `colnames`. Example graphs for features can be coexpression networks, regulatory networks, or co-abundance networks. Example graphs for observations can be cell-cell distances, sample-sample distances, or species networks representing genealogies (as an alternative to phylogenies).

Importantly, node names in each row graph must match `rownames` of the assays, and node names in each column graph must match `colnames` of the assays. Besides, subsetting methods simultaneously subset assays, `rowData`, `rowGraphs`, `colData`, and `colGraphs`.

Besides the constructor function (`GraphExperiment()`), a `GraphExperiment` object can also be created by coercing from a `SummarizedExperiment` or `SingleCellExperiment` object.

Value

A `GraphExperiment` object.

Examples

```
# Example 1: from constructor function ----
## Simulate a matrix with 200 genes and 100 cells
gene_ids <- paste0("gene", seq_len(200))
cell_ids <- paste0("cell", seq_len(100))
mat <- matrix(rpois(20000, 5), ncol = 100, dimnames = list(gene_ids, cell_ids))

## Create a rowGraph from correlations (`igraph` object)
g <- graph_from_adjacency_matrix(cor(t(mat)), weighted = TRUE)

## Create a colGraph, also from correlations (but see scan::buildSNNGraph)
g2 <- graph_from_adjacency_matrix(cor(mat), weighted = TRUE)

## Construct `GraphExperiment` object
ge <- GraphExperiment(
  assays = list(counts = mat),
  rowGraphs = list(cor = g),
  colGraphs = list(cellcor = g2)
)
ge

# Example 2: From `SingleCellExperiment` object ----
sce <- SingleCellExperiment(assays = list(counts = mat))
ge <- as(sce, "GraphExperiment")
ge
```

GraphExperiment-coerce

Coercion methods for GraphExperiment objects

Description

The GraphExperiment class inherits from SingleCellExperiment, which in turn inherits from (Ranged)SummarizedExperiment. To ensure GraphExperiment easily interoperates with these classes, we provide users with traditional as() coercion methods.

Arguments

from An object of class SingleCellExperiment, SummarizedExperiment, or RangedSummarizedExperiment to be coerced to GraphExperiment.

Value

A GraphExperiment object.

Examples

```
# Simulate a count matrix
gene_ids <- paste0("gene", seq_len(200))
cell_ids <- paste0("cell", seq_len(100))
mat <- matrix(rpois(20000, 5), ncol = 100, dimnames = list(gene_ids, cell_ids))

# Coerce from `SummarizedExperiment`
se <- SummarizedExperiment(assays = list(mat))
as(se, "GraphExperiment")

# Coerce from `RangedSummarizedExperiment`
rse <- as(se, "RangedSummarizedExperiment")
as(rse, "GraphExperiment")

# Coerce from `SingleCellExperiment`
sce <- as(se, "SingleCellExperiment")
as(sce, "GraphExperiment")
```

GraphExperiment-methods

Methods for GraphExperiment objects

Description

The GraphExperiment class provides users with methods to get and set graphs (igraph objects) representing how features and observations of SingleCellExperiment objects relate to each other.

Usage

```
## S4 method for signature 'GraphExperiment'  
rowData(x, use.names = TRUE, ...)  
  
## S4 method for signature 'GraphExperiment'  
colData(x, use.names = TRUE, ...)  
  
## S4 method for signature 'GraphExperiment'  
rowGraphs(x)  
  
## S4 method for signature 'GraphExperiment'  
colGraphs(x)  
  
## S4 method for signature 'GraphExperiment,missing'  
rowGraph(x, i)  
  
## S4 method for signature 'GraphExperiment,ANY'  
rowGraph(x, i)  
  
## S4 method for signature 'GraphExperiment,missing'  
colGraph(x, i)  
  
## S4 method for signature 'GraphExperiment,ANY'  
colGraph(x, i)  
  
## S4 method for signature 'GraphExperiment'  
rowGraphNames(x)  
  
## S4 method for signature 'GraphExperiment'  
colGraphNames(x)  
  
## S4 replacement method for signature 'GraphExperiment'  
rowGraphs(x) <- value  
  
## S4 replacement method for signature 'GraphExperiment'  
colGraphs(x) <- value  
  
## S4 replacement method for signature 'GraphExperiment'  
rowGraph(x, i) <- value  
  
## S4 replacement method for signature 'GraphExperiment'  
colGraph(x, i) <- value  
  
## S4 replacement method for signature 'GraphExperiment,character'  
rowGraphNames(x) <- value  
  
## S4 replacement method for signature 'GraphExperiment,character'  
colGraphNames(x) <- value
```

Arguments

<code>x</code>	A GraphExperiment object.
<code>use.names</code>	Passed to the <code>colData</code> method of <code>SingleCellExperiment</code> . Default: <code>TRUE</code> .
<code>...</code>	Ignored.
<code>i</code>	List element (numeric for index, character for name) of the element to access or replace.
<code>value</code>	Replacement value for replacement methods.

Value

Return values depend on the method. See details and examples.

rowGraphs/colGraphs and rowGraph/colGraph methods

`rowGraphs(x)` **and** `colGraphs(x)`: Getter for a `SimpleList` of `igraph` objects representing rows and columns, respectively.

`rowGraphs(x) <- value` **and** `colGraphs(x) <- value`: Setter for a `SimpleList` or list (coerced to `SimpleList`) of `igraph` objects representing rows and columns, respectively.

`rowGraph(x, i)` **and** `colGraph(x, i)`: Getter for an `igraph` object containing graph `i` from the list stored in `rowGraphs` and `colGraphs`, respectively.

`rowGraph(x, i) <- value` **and** `colGraph(x, i) <- value`: Setter for an `igraph` object to be stored in element `i` of `rowGraphs` and `colGraphs`.

rowGraphNames and colGraphNames methods

`rowGraphNames(x)` **and** `colGraphNames(x)`: Getter to extract names of graphs in `rowGraphs` and `colGraphs`.

`rowGraphNames(x) <- value` **and** `colGraphNames(x) <- value`: Setter to assign new names to the graphs stored in `rowGraphs` and `colGraphs`.

rowData method

`rowData(x)`: Getter to extract `rowData` (as in `SingleCellExperiment` objects), but with node attributes of graphs included.

colData method

`colData(x)`: Getter to extract `colData` (as in `SingleCellExperiment` objects), but with node attributes of graphs included.

Examples

```
# Simulate elements of a GraphExperiment object
## Assays
gene_ids <- paste0("gene", seq_len(200))
cell_ids <- paste0("cell", seq_len(100))
mat <- matrix(rpois(20000, 5), ncol = 100, dimnames = list(gene_ids, cell_ids))
```

```
## rowGraph (with node attributes)
g <- graph_from_adjacency_matrix(cor(t(mat)), weighted = TRUE)
V(g)$degree <- igraph::strength(g)

## colGraph
g2 <- graph_from_adjacency_matrix(cor(mat), weighted = TRUE)

## rowData
rdata <- data.frame(
  row.names = gene_ids,
  pathway = sample(c("P1", "P2"), size = length(gene_ids), replace = TRUE),
  coding = sample(c(TRUE, FALSE), size = length(gene_ids), replace = TRUE)
)

## colData
cdata <- data.frame(
  row.names = cell_ids,
  celltype = sample(c("ct1", "ct2"), size = length(cell_ids), replace = TRUE)
)

# Create a GraphExperiment object
ge <- GraphExperiment(
  assays = list(counts = mat),
  rowData = rdata,
  colData = cdata,
  rowGraphs = list(cor = g),
  colGraphs = list(cellcor = g2)
)
ge

# Extract graph names
rowGraphNames(ge)
colGraphNames(ge)

# Extract graphs
rowGraphs(ge)
rowGraph(ge, "cor")

colGraphs(ge)
colGraph(ge, "cellcor")

# Add a new graph
rowGraph(ge, "newcor") <- g
ge

# Add a list of graphs
colGraphs(ge) <- list(cellcor = g2, new_cellcor = g2)
ge
```

```
# Replace graph names
rowGraphNames(ge) <- c("network1", "network2")
ge

# Access rowData (note: rowData + node attributes combined)
rowData(ge)

# Access colData (note: colData + node attributes combined)
colData(ge)
```

GraphExperiment-subset

Subsetting GraphExperiment objects

Description

The subsetting method for [GraphExperiment](#) objects ensures that nodes from [igraph](#) objects are filtered to match rows and columns with the remainder of the object.

Arguments

x	A GraphExperiment object.
i	Numeric, row indices for subsetting.
j	Numeric, column indices for subsetting.

Value

a [GraphExperiment](#) object.

subset

[**:** subsetting method

Examples

```
# Simulate elements of a GraphExperiment object
## Assays
gene_ids <- paste0("gene", seq_len(200))
cell_ids <- paste0("cell", seq_len(100))
mat <- matrix(rpois(20000, 5), ncol = 100, dimnames = list(gene_ids, cell_ids))

## rowGraph (with node attributes)
g <- graph_from_adjacency_matrix(cor(t(mat)), weighted = TRUE)
V(g)$degree <- igraph::strength(g)

## colGraph
g2 <- graph_from_adjacency_matrix(cor(mat), weighted = TRUE)
```

```
## rowData
rdata <- data.frame(
  row.names = gene_ids,
  pathway = sample(c("P1", "P2"), size = length(gene_ids), replace = TRUE),
  coding = sample(c(TRUE, FALSE), size = length(gene_ids), replace = TRUE)
)

## colData
cdata <- data.frame(
  row.names = cell_ids,
  celltype = sample(c("ct1", "ct2"), size = length(cell_ids), replace = TRUE)
)

# Create a GraphExperiment object
ge <- GraphExperiment(
  assays = list(counts = mat),
  rowData = rdata,
  colData = cdata,
  rowGraphs = list(cor = g),
  colGraphs = list(cellcor = g2)
)
ge

# Subset object
ge[1:5, 1:5]
```

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