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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`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(graph)$name`) must match rownames of assays.
`colGraphs`	A list of `igraph` objects with one or multiple graphs representing how observations relate to each other. Node names (i.e., `V(graph)$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 scran::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

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