Package 'tgstat'

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Description A collection of high performance utilities to compute
     distance, correlation, auto correlation, clustering and other tasks.
     Contains graph clustering algorithm described in ``MetaCell: analysis
     of single-cell RNA-seq data using K-nn graph partitions" (Yael Baran,
     Akhiad Bercovich, Arnau Sebe-Pedros, Yaniv Lubling, Amir Giladi, Elad
     Chomsky, Zohar Meir, Michael Hoichman, Aviezer Lifshitz & Amos Tanay,
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tgs_cor

Calculates correlation or auto-correlation

Description

Calculates correlation between two matrices columns or auto-correlation between a matrix columns.

Usage

```
tgs_cor(
  Х,
  y = NULL,
  pairwise.complete.obs = FALSE,
  spearman = FALSE,
  tidy = FALSE,
  threshold = 0
)
tgs_cor_knn(
  Х,
 у,
  knn,
 pairwise.complete.obs = FALSE,
  spearman = FALSE,
  threshold = 0
)
```

Arguments

```
x numeric matrix
y numeric matrix
pairwise.complete.obs
see below
spearman if 'TRUE' Spearman correlation is computed, otherwise Pearson
```

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tidy if 'TRUE' data is outputed in tidy format

threshold absolute threshold above which values are outputed in tidy format

knn the number of highest correlations returned per column

Details

'tgs_cor' is very similar to 'stats::cor'. Unlike the latter it uses all available CPU cores to compute the correlation in a much faster way. The basic implementation of 'pairwise.complete.obs' is also more efficient giving overall great run-time advantage.

Unlike 'stats::cor' 'tgs_cor' implements only two modes of treating data containing NA, which are equivalent to 'use="everything" and 'use="pairwise.complete.obs". Please refer the documentation of this function for more details.

'tgs_cor(x, y, spearman = FALSE)' is equivalent to 'cor(x, y, method = "pearson")' 'tgs_cor(x, y, spearman = TRUE)' is equivalent to 'cor(x, y, method = "spearman")' 'tgs_cor(x, y, pairwise.complete.obs = TRUE, spearman = TRUE)' is equivalent to 'cor(x, y, use = "pairwise.complete.obs", method = "spearman")' 'tgs_cor(x, y, pairwise.complete.obs = TRUE, spearman = FALSE)' is equivalent to 'cor(x, y, use = "pairwise.complete.obs", method = "pearson")'

'tgs_cor' can output its result in "tidy" format: a data frame with three columns named 'col1', 'col2' and 'cor'. Only the correlation values which abs are equal or above the 'threshold' are reported. For auto-correlation (i.e. when 'y=NULL') a pair of columns numbered X and Y is reported only if X < Y.

'tgs_cor_knn' works similarly to 'tgs_cor'. Unlike the latter it returns only the highest 'knn' correlations for each column in 'x'. The result of 'tgs_cor_knn' is always outputed in "tidy" format.

One of the reasons to opt 'tgs_cor_knn' over a pair of calls to 'tgs_cor' and 'tgs_knn' is the reduced memory consumption of the former. For auto-correlation case (i.e. 'y=NULL') given that the number of columns NC exceeds the number of rows NR, then 'tgs_cor' memory consumption becomes a factor of NCxNC. In contrast 'tgs_cor_knn' would consume in the similar scenario a factor of max(NCxNR,NCxKNN). Similarly 'tgs_cor(x,y)' would consume memory as a factor of NCXxNCY, wherever 'tgs_cor_knn(x,y,knn)' would reduce that to max((NCX+NCY)xNR,NCXxKNN).

Value

'tgs_cor_knn' or 'tgs_cor' with 'tidy=TRUE' return a data frame, where each row represents correlation between two pairs of columns from 'x' and 'y' (or two columns of 'x' itself if 'y==NULL'). 'tgs_cor' with the 'tidy=FALSE' returns a matrix of correlation values, where val[X,Y] represents the correlation between columns X and Y of the input matrices (if 'y' is not 'NULL') or the correlation between columns X and Y of 'x' (if 'y' is 'NULL').

```
# Note: all the available CPU cores might be used

set.seed(seed = 0)
rows <- 100
cols <- 1000
vals <- sample(1:(rows * cols / 2), rows * cols, replace = TRUE)
m <- matrix(vals, nrow = rows, ncol = cols)
m[sample(1:(rows * cols), rows * cols / 1000)] <- NA</pre>
```

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```
r1 <- tgs_cor(m, spearman = FALSE)
r2 <- tgs_cor(m, pairwise.complete.obs = TRUE, spearman = TRUE)
r3 <- tgs_cor_knn(m, NULL, 5, spearman = FALSE)</pre>
```

 tgs_dist

Calculates distances between the matrix rows

Description

Calculates distances between the matrix rows.

Usage

```
tgs_dist(x, diag = FALSE, upper = FALSE, tidy = FALSE, threshold = Inf)
```

Arguments

X	numeric	matrix

diag see 'dist' documentation upper see 'dist' documentation

tidy if 'TRUE' data is outputed in tidy format

threshold threshold below which values are outputed in tidy format

Details

This function is very similar to 'package:stats::dist'. Unlike the latter it uses all available CPU cores to compute the distances in a much faster way.

Unlike 'package:stats::dist' 'tgs_dist' uses always "euclidean" metrics (see 'method' parameter of 'dist' function). Thus:

'tgs_dist(x)' is equivalent to 'dist(x, method = "euclidean")'

'tgs_dist' can output its result in "tidy" format: a data frame with three columns named 'row1', 'row2' and 'dist'. Only the distances that are less or equal than the 'threshold' are reported. Distance between row number X and Y is reported only if X < Y. 'diag' and 'upper' parameters are ignored when the result is returned in "tidy" format.

Value

If 'tidy' is 'FALSE' - the output is similar to that of 'dist' function. If 'tidy' is 'TRUE' - 'tgs_dist' returns a data frame, where each row represents distances between two pairs of original rows.

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Examples

```
# Note: all the available CPU cores might be used
set.seed(seed = 0)
rows <- 100
cols <- 1000
vals <- sample(1:(rows * cols / 2), rows * cols, replace = TRUE)
m <- matrix(vals, nrow = rows, ncol = cols)
m[sample(1:(rows * cols), rows * cols / 1000)] <- NA
r <- tgs_dist(m)</pre>
```

tgs_finite

Checks whether all the elements of the vector are finite

Description

Checks whether all the elements of the vector are finite.

Usage

```
tgs_finite(x)
```

Arguments

Х

numeric or integer vector or matrix

Details

```
'tgs_finite' returns 'TRUE' if all the elements of 'x' are finite numbers. (See: 'is.finite'.)
```

Value

'TRUE' if all the elements of 'x' are finite, otherwise 'FALSE'.

```
tgs_finite(1:10)
tgs_finite(c(1:10, NaN))
tgs_finite(c(1:10, Inf))
```

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tgs_graph	Builds directed graph of correlations	

Description

Builds directed graph of correlations where the nodes are the matrix columns.

Usage

```
tgs\_graph(x, knn, k\_expand, k\_beta = 3)
```

Arguments

x see below

knn maximal node degree

k_expand see below k_beta see below

Details

This function builds a directed graph based on the edges in 'x' and their ranks.

'x' is a data frame containing 4 columns named: 'col1', 'col2', 'val', 'rank'. The third column ('val' can have a different name). The result in the compatible format is returned, for example, by 'tgs_knn' function.

'tgs_graph' prunes some of the edges in 'x' based on the following steps:

- 1. A pair of columns i, j that appears in 'x' in 'col1', 'col2' implies the edge in the graph from i to j: edge(i,j). Let the rank of i and j be rank(i,j).
- 2. Calculate symmetrised rank of i and j: $sym_rank(i,j) = rank(i,j) * rank(j,i)$. If one of the ranks is missing from the previous result sym_rank is set to NA.
- 3. Prune the edges: remove edge(i,j) if sym_rank(i,j) == NA OR sym_rank(i,j) < knn * knn * k expand
- 4. Prune excessive incoming edges: remove edge(i,j) if more than knn * k_beta edges of type edge(node,j) exist and sym_rank(i,j) is higher than sym_rank(node,j) for node != j.
- 5. Prune excessive outgoing edges: remove edge(i,j) if more than knn edges of type edge(i,node) exist and sym_rank(i,j) is higher than sym_rank(i,node) for node != i.

Value

The graph edges are returned in a data frame, with the weight of each edge. edge(i,j) receives weight 1 if its sym_rank is the lowest among all edges of type edge(i,node). Formally defined: weight(i,j) = 1 - (place(i,j) - 1) / knn, where place(i,j) is the location of edge(i,j) within the sorted set of edges outgoing from i, i.e. edge(i,node). The sort is done by sym_rank of the edges.

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Examples

```
# Note: all the available CPU cores might be used

set.seed(seed = 1)
rows <- 100
cols <- 1000
vals <- sample(1:(rows * cols / 2), rows * cols, replace = TRUE)
m <- matrix(vals, nrow = rows, ncol = cols)
m[sample(1:(rows * cols), rows * cols / 1000)] <- NA

r1 <- tgs_cor(m, pairwise.complete.obs = FALSE, spearman = TRUE)
r2 <- tgs_knn(r1, knn = 30, diag = FALSE)
r3 <- tgs_graph(r2, knn = 3, k_expand = 10)</pre>
```

tgs_graph_cover

Clusters directed graph

Description

Clusters directed graph.

Usage

```
tgs_graph_cover(graph, min_cluster_size, cooling = 1.05, burn_in = 10)
```

Arguments

```
graph directed graph in the format returned by tgs_graph

min_cluster_size

used to determine the candidates for seeding (= min weight)

cooling factor that is used to gradually increase the chance of a node to stay in the cluster burn_in number of node reassignments after which cooling is applied
```

Details

The algorithm is explained in a "MetaCell: analysis of single-cell RNA-seq data using K-nn graph partitions" paper, published in "Genome Biology" #20: https://genomebiology.biomedcentral.com/articles/10.1186/s13059-019-1812-2

Value

Data frame that maps each node to its cluster.

See Also

```
tgs_graph()
```

Examples

```
# Note: all the available CPU cores might be used

set.seed(seed = 0)
rows <- 100
cols <- 1000
vals <- sample(1:(rows * cols / 2), rows * cols, replace = TRUE)
m <- matrix(vals, nrow = rows, ncol = cols)
m[sample(1:(rows * cols), rows * cols / 1000)] <- NA

r1 <- tgs_cor(m, pairwise.complete.obs = FALSE, spearman = TRUE)
r2 <- tgs_knn(r1, knn = 30, diag = FALSE)
r3 <- tgs_graph(r2, knn = 3, k_expand = 10)
r4 <- tgs_graph_cover(r3, 5)</pre>
```

```
tgs_graph_cover_resample
```

Clusters directed graph multiple times with randomized sample subset

Description

Clusters directed graph multiple times with randomized sample subset.

Usage

```
tgs_graph_cover_resample(
  graph,
  knn,
  min_cluster_size,
  cooling = 1.05,
  burn_in = 10,
  p_resamp = 0.75,
  n_resamp = 500,
  method = "hash"
)
```

Arguments

graph directed graph in the format returned by tgs_graph
knn maximal number of edges used per node for each sample subset

```
min_cluster_size

used to determine the candidates for seeding (= min weight)

cooling

factor that is used to gradually increase the chance of a node to stay in the cluster burn_in

number of node reassignments after which cooling is applied

p_resamp

fraction of total number of nodes used in each sample subset

n_resamp

number iterations the clustering is run on different sample subsets

method

method for calculating co_cluster and co_sample; valid values: "hash", "full", "edges"
```

Details

The algorithm is explained in a "MetaCell: analysis of single-cell RNA-seq data using K-nn graph partitions" paper, published in "Genome Biology" #20: https://genomebiology.biomedcentral.com/articles/10.1186/s13059-019-1812-2

Value

If method == "hash", a list with two members. The first member is a data frame with 3 columns: "node1", "node2" and "cnt". "cnt" indicates the number of times "node1" and "node2" appeared in the same cluster. The second member of the list is a vector of **number of nodes** length reflecting how many times each node was used in the subset.

```
If method == "full", a list containing two matrices: co_cluster and co_sample.
```

If method == "edges", a list containing two data frames: co_cluster and co_sample.

See Also

```
tgs_graph()
```

```
# Note: all the available CPU cores might be used

set.seed(seed = 0)
rows <- 100
cols <- 200
vals <- sample(1:(rows * cols / 2), rows * cols, replace = TRUE)
m <- matrix(vals, nrow = rows, ncol = cols)

r1 <- tgs_cor(m, pairwise.complete.obs = FALSE, spearman = TRUE)
r2 <- tgs_knn(r1, knn = 20, diag = FALSE)
r3 <- tgs_graph(r2, knn = 3, k_expand = 10)
r4 <- tgs_graph_cover_resample(r3, 10, 1)</pre>
```

10 tgs_knn

Returns k highest values of each column

Description

Returns k highest values of each column.

Usage

```
tgs_knn(x, knn, diag = FALSE, threshold = 0)
```

Arguments

x numeric matrix or data frame (see below)

knn the number of highest values returned per column

diag if 'F' values of row 'i' and col 'j' are skipped for each i == j

threshold filter out values lower than threshold

Details

'tgs_knn' returns the highest 'knn' values of each column of 'x' (if 'x' is a matrix). 'x' can be also a sparse matrix given in a data frame of 'col', 'row', 'value' format.

'NA' and 'Inf' values are skipped as well as the values below 'threshold'. If 'diag' is 'F' values of the diagonal (row == col) are skipped too.

Value

A sparse matrix in a data frame format with 'col1', 'col2', 'val' and 'rank' columns. 'col1' and 'col2' represent the column and the row number of 'x'.

```
# Note: all the available CPU cores might be used

set.seed(seed = 1)
rows <- 100
cols <- 1000
vals <- sample(1:(rows * cols / 2), rows * cols, replace = TRUE)
m <- matrix(vals, nrow = rows, ncol = cols)
m[sample(1:(rows * cols), rows * cols / 1000)] <- NA
r <- tgs_knn(m, 3)</pre>
```

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tgs_matrix_tapply

For each matrix row apply a function over a ragged array

Description

For each matrix row apply a function to each cell of a ragged array, that is to each (non-empty) group of values given by a unique combination of the levels of certain factors.

Usage

```
tgs_matrix_tapply(x, index, fun, ...)
```

Arguments

X	a matrix or a sparse matrix of 'dgCMatrix' type
index	a 'list' of one or more 'factor's, each of same length as the number of columns in 'x'. The elements are coerced to factors by 'as.factor'.
fun	the function to be applied
	optional arguments to 'fun'

Details

'tgs_matrix_tapply(x, index, fun)' is essentialy an efficient implementation of 'apply(mat, 1, function(x) tapply(x, index, fun))'.

Value

A matrix of length(index) X nrow(x) size. Each [i,j] element represents the result of applying 'fun' to x[i,which(index==levels(index)[j])].

Note that the return value is a dense matrix even when x is sparse.

```
# Note: all the available CPU cores might be used

set.seed(seed = 1)
nr <- 6
nc <- 10
mat <- matrix(sample(c(rep(0, 6), 1:3), nr * nc, replace = TRUE), nrow = nr, ncol = nc)
index <- factor(rep_len(1:3, ncol(mat)), levels = 0:5)
r1 <- apply(mat, 1, function(x) tapply(x, index, sum))
r2 <- tgs_matrix_tapply(mat, index, sum)</pre>
```

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