Package 'scellpam'

January 9, 2023

Type Package **Title** Applying Partitioning Around Medoids to Single Cell Data with High Number of Cells Version 1.4.1 **Author** Juan Domingo [aut, cre] (https://orcid.org/0000-0003-4728-6256), Guillermo Ayala [ctb] (https://orcid.org/0000-0002-6231-2865">https://orcid.org/0000-0002-6231-2865), Spanish Ministry of Science and Innovation, MCIN/AEI <doi:10.13039/501100011033> [fnd] Maintainer Juan Domingo < Juan. Domingo@uv.es> Description PAM (Partitioning Around Medoids) algorithm application to samples of single cell sequencing techniques with a high number of cells (as many as the computer memory allows). The package uses a binary format to store matrices (either full, sparse or symmetric) in files written in the disk that can contain any data type (not just double) which allows its manipulation when memory is sufficient to load them as int or float, but not as double. The PAM implementation is done in parallel, using several/all the cores of the machine, if it has them. This package shares a great part of its code with packages 'jmatrix' and 'parallelpam' but their functionality is included here so there is no need to install them. License GPL (>= 2)**Imports** Rcpp (>= 1.0.8), memuse (>= 4.2.1), cluster (>= 2.1.4) LinkingTo Rcpp SystemRequirements C++14 RoxygenNote 7.2.1 **Encoding UTF-8** Suggests rmarkdown, knitr, DuoClustering2018, scater, splatter VignetteBuilder knitr **NeedsCompilation** yes

Repository CRAN

Date/Publication 2023-01-09 08:10:02 UTC

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Description

A function to implement the Partitioning-around-medoids algorithm described in

Schubert, E. and Rousseeuw, P.J.: "Fast and eager k-medoids clustering: O(k) runtime improvement of the PAM, CLARA, and CLARANS algorithms."

Information Systems, vol. 101, p. 101804, 2021.

doi: https://doi.org/10.1016/j.is.2021.101804

Notice that the actual values of the vectors (instances) are not needed. To recover them, look at the data matrix used to generate the distance matrix.

The number of instances, N, is not passed since dissimilarity matrix is NxN and therefore its size indicates the N value.

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Usage

```
ApplyPAM(
   dissim_file,
   k,
   init_method = "BUILD",
   initial_med = NULL,
   max_iter = 1000L,
   nthreads = 0L
)
```

Arguments

dissim_file A string with the name of the binary file that contains the symmetric matrix

of dissimilarities. Such matrix should have been generated by CalcAndWrite-DissimilarityMatrix and it is a matrix of type 'disttype' (in this type defined as

float).

k A possitive integer (the desired number of medoids).

init_method One of the strings 'PREV', 'BUILD' or 'LAB'. See meaning of initialization

algorithms BUILD and LAB in the original paper.

'PREV' should be used exclusively to start the second part of the algorithm

(optimization) from a initial set of medoids generated by a former call.

Default: BUILD.

initial_med A vector with initial medoids to start optimization. It is to be used only by the

'PREV' method and it will have been obtained as the first element (L\$med) of the two-element list returned by a previous call to this function used in just-

initialize mode (max_iter=0).

Default: empty vector.

max_iter The maximum number of allowed iterations. 0 means stop immediately after

finding initial medoids.

Default: 1000

nthreads For the BUILD initialization algorithm (the only part currently implemented in

parallel), the number of used threads.

-1 means don't use threads (serial implementation). 0 means let the program

choose according to the number of cores and of points.

Any other number forces this number of threads. Choosing more than the num-

ber of available cores is allowed, but discouraged.

Default: 0

Details

With respect to the returned value, L\$med has as many components as requested medoids and L\$clasif has as many components as instances.

Medoids are expressed in L\$med by its number in the array of points (row in the dissimilarity matrix) starting at 1 (R convention).

L\$clasif contains the number of the medoid (i.e.: the cluster) to which each instance has been assigned, according to their order in

L\$med (also from 1).

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This means that if L\$clasif[p] is m, the point p belongs to the class grouped around medoid L\$med[m].

Moreover, if the dissimilarity matrix contains as metadata the point names, the returned are R-named vector with such names.

Value

L["med", "clasif"] A list of two numeric vectors. See section Details for more information

Examples

```
# Synthetic problem: 10 random seeds with coordinates in [0..20]
# to which random values in [-0.1..0.1] are added
M<-matrix(0,100,500)
rownames(M)<-paste0("rn",c(1:100))</pre>
for (i in (1:10))
 p<-20*runif(500)
 Rf <- matrix(0.2*(runif(5000)-0.5),nrow=10)
 for (k in (1:10))
 M[10*(i-1)+k,]=p+Rf[k,]
 }
tmpfile1=paste0(tempdir(),"/pamtest.bin")
JWriteBin(M, tmpfile1, dtype="float", dmtype="full")
tmpdisfile1=paste0(tempdir(),"/pamDL2.bin")
CalcAndWriteDissimilarityMatrix(tmpfile1,tmpdisfile1,distype="L2",restype="float",nthreads=0)
L <- ApplyPAM(tmpdisfile1,10,init_method="BUILD")</pre>
# Final value of sum of distances to closest medoid
GetTD(L,tmpdisfile1)
# Medoids:
L$med
# Medoid in which each individual has been classified
n<-names(L$med)</pre>
n[L$clasif]
```

BuildAbundanceMatrix BuildAbundanceMatrix

Description

Builds and returns a R matrix with as many rows as clusters and as many columns as groups in the set of cells (individuals). The entry at row r, column c is the number if individuals of group c which the classifier has identified as belonging to cluster r

```
BuildAbundanceMatrix(clasif, gr, expgroups = 0L)
```

Arguments

clasif The vector with the number of the cluster each cell belongs to. Usually ob-

tained as L\$clasif, being L the object returned by ApplyPAM. It MUST be a vector of integers with as many components as cells and values in (1..number_of_clusters). Obviously, it can be a named vector but the group names are

not used.

gr A numeric vector with the group (of those designed for the assay) to which each

cell belongs to. Normally obtained with GetSeuratGroups if the assay is in Seurat format. Otherwise, you will have to provide it yourself. It MUST be vector of integers with as many components as cells and values in (1..number_of_groups).

Obviously, it can be a named vector but the cell names are not used.

expgroups The expected number of groups. If it is left to its default value (which is 0) the

number of groups is infered from parameter grname as the maximum value in it. Otherwise, the passed value is used. This parameter is to prevent the extinction of some groups due to previous expurge or filtering but whose trail we want to

keep, even they are currently empty.

Value

M(numclusters,numgroups) A R matrix as many rows as clusters and as many columns as groups

Examples

Sorry, we can't provide examples here since they require the application to a real problem # and therefore the load of the Seurat or splatter packages. Please, look at example in the # vignette of this package.

CalcAndWriteDissimilarityMatrix

 ${\it CalcAndWriteDissimilarityMatrix}$

Description

Writes a binary symmetric matrix with the dissimilarities between ROWS of the data stored in a binary matrix in the scellpam package format.

Notice that, differently from the common practice in single cell, the rows represent cells. This is for efficiency reasons and it is transparent to the user, as long as he/she has generated the binary matrix (with CsvToBinMat, dgCMatToBinMat or SceToBinMat) using the option transpose=TRUE.

The input matrix of vectors can be a full or a sparse matrix. Output matrix type can be float or double type (but look at the comments in 'Details').

```
CalcAndWriteDissimilarityMatrix(
  ifname,
  ofname,
```

```
distype = "L2",
  restype = "float",
  comment = "",
  nthreads = 0L
)
```

Arguments

ifname	A string with the name of the file containing the counts as a binary matrix, as written by CsvToBinMat, dgCMatToBinMat or SceToBinMat
ofname	A string with the name of the binary output file to contain the symmetric dissimilarity matrix.
distype	The dissimilarity to be calculated. It must be one of these strings: $^{\prime}L1^{\prime}$, $^{\prime}L2^{\prime}$ or $^{\prime}Pearson^{\prime}$. Default: $^{\prime}L2^{\prime}$.
restype	The data type of the result. It can be one of the strings 'float' or 'double'. Default: float (and don't change it unless you REALLY need to).
comment	Comment to be added to the dissimilary matrix. Default: "" (no comment)
nthreads	Number of threads to be used for the parallel calculations with this meaning: -1: don't use threads. 0: let the function choose according to the number of individuals (cells) and to the number of available cores.
	Any possitive number > 1: use that number of threads. You can use even more than cores, but this is discouraged and raises a warning. Default: 0.

Details

The parameter restype forces the output to be a matrix of either floats or doubles. Precision of float if normally good enough; but if you need double precision (may be because you expect your results to be in a large range, two to three orders of magnitude), change it.

Nevertheless, notice that this at the expense of double memory usage, which is QUADRATIC with the number of individuals (rows) in your input matrix.

Value

No return value, called for side effects (creates a file)

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CalculateSilhouette

CalculateSilhouette

Description

Calculates the silhouette of each point of those classified by a clustering algorithm.

Usage

```
CalculateSilhouette(cl, fdist, nthreads = 0L)
```

Arguments

cl The array of classification with the number of the class to which each point be-

longs to. This number must be in 1..number_of_classes.

This function takes something like the L\$clasif array which is the second ele-

ment of the list returned by ApplyPAM

fdist The binary file containing the symmetric matrix with the dissimilarities between

points (usually, generated by a call to CalcAndWriteDissimilarityMatrix)

nthreads The number of used threads.

-1 means don't use threads (serial implementation). 0 means let the program

choose according to the number of cores and of points.

Any other number forces this number of threads. Choosing more than the num-

ber of available cores is allowed, but discouraged.

Default: 0

Value

sil Numeric vector with the values of the silhouette for each point, in the same order in which points

If cl is a named vector sill will be a named vector, too, with the same names.

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Examples

```
# Synthetic problem: 10 random seeds with coordinates in [0..20]
# to which random values in [-0.1..0.1] are added
M<-matrix(0,100,500)
rownames(M)<-paste0("rn",c(1:100))</pre>
for (i in (1:10))
 p<-20*runif(500)
 Rf <- matrix(0.2*(runif(5000)-0.5), nrow=10)
 for (k in (1:10))
 M[10*(i-1)+k,]=p+Rf[k,]
 }
tmpfile1=paste0(tempdir(),"/pamtest.bin")
JWriteBin(M, tmpfile1, dtype="float", dmtype="full")
tmpdisfile1=paste0(tempdir(),"/pamDL2.bin")
CalcAndWriteDissimilarityMatrix(tmpfile1,tmpdisfile1,distype="L2",restype="float",nthreads=0)
L <- ApplyPAM(tmpdisfile1,10,init_method="BUILD")</pre>
sil <- CalculateSilhouette(L$clasif,tmpdisfile1)</pre>
# Histogram of the silhouette. In this synthetic problem, almost 1 for all points
hist(sil)
```

ClassifAsDataFrame

ClassifAsDataFrame

Description

Returns the results of the classification returned by ApplyPAM as a R dataframe

Usage

```
ClassifAsDataFrame(L, fdist)
```

Arguments

L The list returned by ApplyPAM with fields L\$med and

L\$clasif with the numbers of the medoids and the classification of each point

fdist The binary file containing the symmetric matrix with the dissimilarities between

points (usually, generated by a call to CalcAndWriteDissimilarityMatrix or to

CalcAndWriteDissimilarityMatrixDouble)

Details

The dataframe has three columns: PointName (name of each point), NNPointName (name of the point which is the center of the cluster to which PointName belongs to) and NNDistance (distance between the points PointName and NNPointName). Medoids are identified by the fact that PointName and NNPointName are equal, or equivalently, NNDistance is 0.

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Value

Df Dataframe with columns PointName, NNPointName and NNDistance. See Details for description

Examples

```
# Synthetic problem: 10 random seeds with coordinates in [0..20]
# to which random values in [-0.1..0.1] are added
M<-matrix(0,100,500)
rownames(M)<-paste0("rn",c(1:100))</pre>
for (i in (1:10))
 p<-20*runif(500)
 Rf <- matrix(0.2*(runif(5000)-0.5),nrow=10)
 for (k in (1:10))
  M[10*(i-1)+k,]=p+Rf[k,]
 }
}
tmpfile1=paste0(tempdir(),"/pamtest.bin")
JWriteBin(M,tmpfile1,dtype="float",dmtype="full")
tmpdisfile1=paste0(tempdir(),"/pamDL2.bin")
CalcAndWriteDissimilarityMatrix(tmpfile1,tmpdisfile1,distype="L2",restype="float",nthreads=0)
L <- ApplyPAM(tmpdisfile1,10,init_method="BUILD")</pre>
df <- ClassifAsDataFrame(L,tmpdisfile1)</pre>
df
# Identification of medoids:
which(df[,3]==0)
\# Verification they are the same as in L (in different order)
L$med
```

CsvToJMat

CsvToJMat

Description

Gets a csv file and writes to a disk file the binary matrix of counts contained in it in the jmatrix binary format.

First line of the .csv is supposed to have the field names.

First column of each line is supposed to have the field name.

The fields are supposed to be separated by one occurrence of a character-field sepparator (usually, comma or tab)

```
CsvToJMat(
  ifname,
  ofname,
  mtype = "sparse",
```

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```
csep = ",",
ctype = "raw",
valuetype = "float",
transpose = FALSE,
comment = ""
)
```

Arguments

ifname A string with the name of the .csv text file.

ofname A string with the name of the binary output file.

mtype A string to indicate the matrix type: 'full' or 'sparse'. Default: 'sparse' csep The character used as separator in the .csv file. Default: ',' (comma)

ctype The string 'raw' or 'log1' to write raw counts or log(counts+1), or the normal-

ized versions, 'rawn' and 'log1n', which normalize ALWAYS BY COLUMNS (before transposition, if requested to transpose). The logarithm is taken base 2.

Default: raw

valuetype The data type to store the matrix. It must be one of the strings 'uint32', 'float'

or 'double'. Default: float

transpose Boolean to indicate if the matrix should be transposed before writing. See De-

tails for a comment about this. Default: FALSE

comment A comment to be stored with the matrix. Default: "" (no comment)

Details

The parameter transpose has the default value of FALSE. But don't forget to set it to TRUE if you want the cells (which in single cell common practice are by columns) to be written by rows. This will be needed later to calculate the dissimilarity matrix, if this is the next step of your workflow. See help of CalcAndWriteDissimilarityMatrix

Value

No return value, called for side effects (creates a file)

```
# Since we have no a .csv file to test, we will generate one with another funcion of this package
Rf <- matrix(runif(48),nrow=6)
rownames(Rf) <- c("A","B","C","D","E","F")
colnames(Rf) <- c("a","b","c","d","e","f","g","h")
tmpfile1=paste0(tempdir(),"/Rfullfloat.bin")
tmpfile2=paste0(tempdir(),"/Rfullfloat2.bin")
tmpcsvfile1=paste0(tempdir(),"/Rfullfloat.csv")
JWriteBin(Rf,tmpfile1,dtype="float",dmtype="full",comment="Full matrix of floats")
JMatToCsv(tmpfile1,tmpcsvfile1)
CsvToJMat(tmpcsvfile1,tmpfile2)
# It can be checked that files Rfullfloat.bin and Rfullfloat2.bin contain the same data
# (even hey differ in the comment, which has been eliminated when converting to csv)</pre>
```

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dgCMatToJMat	dgCMatToJMat	

Description

Gets a dgCMatrix object and writes to a disk file the binary matrix of counts contained in it in the jmatrix binary format. Plase, see Details below to know more about the extraction of the sparse matrices from Seurat or similar single cell formats.

Usage

```
dgCMatToJMat(
   q,
   fname,
   mtype = "sparse",
   ctype = "raw",
   valuetype = "float",
   transpose = FALSE,
   comment = ""
)
```

Arguments

q	The dgCMatrix object
fname	A string with the name of the binary output file
mtype	A string to indicate the matrix type: 'full' or 'sparse'. Default: 'sparse'
ctype	The string 'raw' or 'log1' to write raw counts or log(counts+1), or the normalized versions, 'rawn' and 'log1n', which normalize ALWAYS BY COLUMNS (before transposition, if requested to transpose). Default: raw
valuetype	The data type to store the matrix. It must be one of the strings 'uint32', 'float' or 'double'. Default: float
transpose	Boolean to indicate if the matrix should be transposed before writing. See Details for a comment about this. Default: FALSE
comment	A comment to be stored with the matrix. Default: "" (no comment)

Details

We have found that, in some Seurat objects, the dgCMatrix to be passed to this function can be extracted as q@assays\$RNA@counts, being q the Seurat S4 object.

In other cases this matrix is obtained as q@raw.data.

In any case, we assume that this matrix has slots Dimnames (with a list of strings in Dimnames[[0]] as rownames and Dimnames[[1]] as column names) as long as slots with names i, p and x as described in the documentation of the R Matrix library on sparse matrices.

The parameter transpose has the default value of FALSE. But don't forget to set it to TRUE if you want the cells (which in single cell common practice are by columns) to be written by rows. This will be needed later to calculate the dissimilarity matrix, if this is the next step of your workflow. See help of CalcAndWriteDissimilarityMatrix

Value

No return value, called for side effects (creates a file)

Examples

```
# Sorry, we cannot provide an example here, since it would need the load of the Seurat package. # Please, see the vignette for examples
```

```
{\tt FilterBySilhouetteQuantile}
```

Filter By Silhou ette Quantile

Description

Takes a silhouette, as returned by CalculateSilhouette, the list of medoids and class assignments, as returned by ApplyPam, a quantile and the matrices of counts and dissimilarities and constructs the corresponding matrices clearing off the points (cells) whose silhoutte is below the lower quantile, except if they are medoids.

Usage

```
FilterBySilhouetteQuantile(
    s,
    L,
    fallcounts,
    ffilcounts,
    falldissim,
    ffildissim,
    q = 0.2,
    addcom = TRUE
)
```

Arguments

S	A numeric vector with the sihouette coefficient of each point (cell) in a classification, as returned by CalculateSilhouette.
L	A list of two numeric vectors, L\$med and L\$clasif, obtained normally as the object returned by ApplyPAM.
fallcounts	A string with the name of the binary file containing the matrix of counts per cell. It can be either a full or a sparse matrix.
ffilcounts	A string with the name of the binary file that will contain the selected cells. It will have the same character (full/sparse) and type of the complete file.
falldissim	A string with the name of the binary file containing the dissimilarity matrix of the complete set of cells. It must be a symmetric matrix of floats.

ffildissim A string with the name of the binary file that will contain the dissimilarity matrix for the remaining cells. It will be a symmetric matrix of floats.

Quantile to filter. All points (cells) whose silhouette is below this quantile will

be filtered out. Default: 0.2

addcom Boolean to indicate if a comment must be appended to the current comment of

counts and dissimilarity matrices to indicate that they are the result of a filtering process. This comment is automatically generated and contains the value of quantile q. Succesive applications add comments at the end of those already

present. Default: TRUE

Details

q

The renumbering of indices in the returned cluster may seem confusing at first but it was the way of fitting this with the rest of the package. Anyway, notice that if the numeric vectors in the input parameter L were named vectors, the cells names are appropriately kept in the result so cell identity is preserved. Moreover, if the counts and dissimilarity input matrices had row and/or column names, they are preserved in the filtered matrices, too.

Value

Lr["med","clasif"] A list of two numeric vectors.

Lr\$med is a modification of the correponding first element of the passed L parameter.

Lr\$clasif has as many components as remaining instances.

Since points (cells) will have been removed, medoid numbering is modified. Therefore, Lr\$med has the NEW index of each medoid in the filtered set.

Lr\$clasif contains the number of the medoid (i.e.: the cluster) to which each instance has been assigned, and therefore does not change.

All indexes start at 1 (R convention). Please, see Details section

```
# Synthetic problem: 10 random seeds with coordinates in [0..20]
# to which random values in [-0.1..0.1] are added
M<-matrix(0,100,500)
rownames(M)<-paste0("rn",c(1:100))
for (i in (1:10))
{
    p<-20*runif(500)
    Rf <- matrix(0.2*(runif(5000)-0.5),nrow=10)
    for (k in (1:10))
    {
        M[10*(i-1)+k,]=p+Rf[k,]
    }
}
tmpfile1=paste0(tempdir(),"/pamtest.bin")
JWriteBin(M,tmpfile1,dtype="float",dmtype="full")
tmpdisfile1=paste0(tempdir(),"/pamD12.bin")
CalcAndWriteDissimilarityMatrix(tmpfile1,tmpdisfile1,distype="L2",restype="float",nthreads=0)
L <- ApplyPAM(tmpdisfile1,10,init_method="BUILD")</pre>
```

FilterBySilhouetteThreshold

FilterBySilhouetteThreshold

Description

Takes a silhouette, as returned by CalculateSilhouette, the list of medoids and class assignments, as returned by ApplyPam, a threshold and the matrices of counts and dissimilarities and constructs the corresponding matrices clearing off the points (cells) whose silhoutte is below the threshold, except if they are medoids.

Usage

```
FilterBySilhouetteThreshold(
    s,
    L,
    fallcounts,
    ffilcounts,
    falldissim,
    ffildissim,
    thres = 0,
    addcom = TRUE
)
```

Arguments

S	A numeric vector with the sihouette coefficient of each point in a classification, as returned by CalculateSilhouette.
L	A list of two numeric vectors, L\$med and L\$clasif, obtained normally as the object returned by ApplyPAM.
fallcounts	A string with the name of the binary file containing the matrix of counts per cell. It can be either a full or a sparse matrix.
ffilcounts	A string with the name of the binary file that will contain the selected cells. It will have the same character (full/sparse) and type of the complete file.
falldissim	A string with the name of the binary file containing the dissimilarity matrix of the complete set of cells. It must be a symmetric matrix of floats.

ffildissim A string with the name of the binary file that will contain the dissimilarity matrix

for the remaining cells. It will be a symmetric matrix of floats.

thres Threshold to filter. All points whose silhouette is below this threshold will be

filtered out. Default: 0.0 (remember that silhouette is in [-1..1])

addcom Boolean to indicate if a comment must be appended to the current comment of

counts and dissimilarity matrices to indicate that they are the result of a filtering process. This comment is automatically generated and contains the value of threshold t. Succesive applications add comments at the end of those already

present. Default: TRUE

Details

The renumbering of indices in the returned cluster may seem confusing at first but it was the way of fitting this with the rest of the package. Anyway, notice that if the numeric vectors in the input parameter L were named vectors, the cells names are appropriately kept in the result so cell identity is preserved. Moreover, if the counts and dissimilarity input matrices had row and/or column names, they are preserved in the filtered matrices, too.

Value

Lr["med","clasif"] A list of two numeric vectors.

Lr\$med is a modification of the correponding first element of the passed L parameter.

Lr\$clasif has as many components as remaining instances.

Since points will have been removed, medoid numbering is modified. Therefore, Lr\$med has the NEW index of each medoid in the filtered set.

Lr\$clasif contains the number of the medoid (i.e.: the cluster) to which each instance has been assigned, and therefore does not change.

All indexes start at 1 (R convention). Please, see Details section

```
# Synthetic problem: 10 random seeds with coordinates in [0..20]
# to which random values in [-0.1..0.1] are added
M<-matrix(0,100,500)
rownames(M)<-paste0("rn",c(1:100))
for (i in (1:10))
{
    p<-20*runif(500)
    Rf <- matrix(0.2*(runif(5000)-0.5),nrow=10)
    for (k in (1:10))
    {
        M[10*(i-1)+k,]=p+Rf[k,]
    }
}
tmpfile1=paste0(tempdir(),"/pamtest.bin")
JWriteBin(M,tmpfile1,dtype="float",dmtype="full")
tmpdisfile1=paste0(tempdir(),"/pamD12.bin")
CalcAndWriteDissimilarityMatrix(tmpfile1,tmpdisfile1,distype="L2",restype="float",nthreads=0)
L <- ApplyPAM(tmpdisfile1,10,init_method="BUILD")</pre>
```

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FilterJMatByName

FilterJMatByName

Description

Takes a jmatrix binary file containing a table with cells and genes and filter the genes or cell by name, eliminating those whose names are not in certain list

Usage

```
FilterJMatByName(fname, Gn, filname, namesat = "rows")
```

Arguments

fname A string with the file name of the original table

Gn A list of R strings with the names of the genes or cells that must remain. All

others will be filtered out

filname A string with the file name of the filtered table

namesat The string "rows" or "cols" indicating if the genes/cells at the original table are

by rows or by colums. Default: "rows"

Details

If the table has no list of names in the requested dimension (rows or colums), an error is rised.

The gene or cell names whose names are not found obviosuly cannot remain, and the program rises a warning indicating for which gene/cell names this happens.

The matrix contained in the filtered file will have the same nature (full or sparse) and the same data type as the original.

This function can be used to filter either by cell or by gene name, with appropriate usage of parameter namesat

Value

No return value, called for side effects (creates a file)

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Examples

```
Rf <- matrix(runif(48),nrow=6)</pre>
rownames(Rf) <- c("A", "B", "C", "D", "E", "F")
colnames(Rf) <- c("a","b","c","d","e","f","g","h")</pre>
tmpfile1=paste0(tempdir(),"/Rfullfloat.bin")
tmpfile2=paste0(tempdir(),"/Rfullfloatrowfilt.bin")
tmpfile3=paste0(tempdir(),"/Rfullfloatrowcolfilt.bin")
tmpcsvfile1=paste0(tempdir(),"/Rfullfloat.csv")
tmpcsvfile3=paste0(tempdir(),"/Rfullfloatrowcolfilt.csv")
JWriteBin(Rf,tmpfile1,dtype="float",dmtype="full",comment="Full matrix of floats")
# Let's keep only rows A, C and E
FilterJMatByName(tmpfile1,c("A","C","E"),tmpfile2,namesat="rows")
\mbox{\tt\#} and from the result, let's keep only columns b, d and g
FilterJMatByName(tmpfile2,c("b","d","g"),tmpfile3,namesat="cols")
JMatToCsv(tmpfile1,tmpcsvfile1)
JMatToCsv(tmpfile3,tmpcsvfile3)
# You can now compare both ASCII/csv files
```

GetJCol

GetJCol

Description

Returns (as a R numeric vector) the requested column number from the matrix contained in a jmatrix binary file

Usage

```
GetJCol(fname, ncol)
```

Arguments

fname String with the file name that contains the binary data.

ncol The number of the column to be returned, in R-numbering (from 1)

Value

A numeric vector with the values of elements in the requested column

```
Rf <- matrix(runif(48),nrow=6)
rownames(Rf) <- c("A","B","C","D","E","F")
colnames(Rf) <- c("a","b","c","d","e","f","g","h")
tmpfile1=paste0(tempdir(),"/Rfullfloat.bin")
JWriteBin(Rf,tmpfile1,dtype="float",dmtype="full",comment="Full matrix of floats")
Rf[,3]
vf<-GetJCol(tmpfile1,3)
vf</pre>
```

18 GetJColNames

GetJColByName

GetJColByName

Description

Returns (as a R numeric vector) the requested named column from the matrix contained in a jmatrix binary file

Usage

```
GetJColByName(fname, colname)
```

Arguments

fname String with the file name that contains the binary data.

colname The name of the column to be returned. If the matrix has no column names, or

the name is not found, an empty vector is returned

Value

A numeric vector with the values of elements in the requested column

Examples

```
Rf <- matrix(runif(48),nrow=6)
rownames(Rf) <- c("A","B","C","D","E","F")
colnames(Rf) <- c("a","b","c","d","e","f","g","h")
tmpfile1=paste0(tempdir(),"/Rfullfloat.bin")
JWriteBin(Rf,tmpfile1,dtype="float",dmtype="full",comment="Full matrix of floats")
Rf[,"c"]
vf<-GetJColByName(tmpfile1,"c")
vf</pre>
```

GetJColNames

GetJColNames

Description

Returns a R StringVector with the column names of a matrix stored in the binary format of package jmatrix, if it has them stored.

```
GetJColNames(fname)
```

GetJManyCols 19

Arguments

fname String with the file name that contains the binary data.

Value

A R StringVector with the column names, or the empty vector if the binaryfile has no row column names as metadata.

Examples

```
Rf <- matrix(runif(48),nrow=6)
rownames(Rf) <- c("A","B","C","D","E","F")
colnames(Rf) <- c("a","b","c","d","e","f","g","h")
tmpfile1=paste0(tempdir(),"/Rfullfloat.bin")
JWriteBin(Rf,tmpfile1,dtype="float",dmtype="full",comment="Full matrix of floats")
cn<-GetJColNames(tmpfile1)
cn</pre>
```

GetJManyCols

GetJManyCols

Description

Returns (as a R numeric matrix) the columns with the requested column numbers from the matrix contained in a jmatrix binary file

Usage

```
GetJManyCols(fname, extcols)
```

Arguments

fname String with the file name that contains the binary data.

extcols A numeric vector with the indexes of the columns to be extracted, in R-numbering

(from 1)

Value

A numeric matrix with the values of elements in the requested columns

```
Rf <- matrix(runif(48),nrow=6)
rownames(Rf) <- c("A","B","C","D","E","F")
colnames(Rf) <- c("a","b","c","d","e","f","g","h")
tmpfile1=paste0(tempdir(),"/Rfullfloat.bin")
JWriteBin(Rf,tmpfile1,dtype="float",dmtype="full",comment="Full matrix of floats")
vc<-GetJManyCols(tmpfile1,c(1,4))
vc</pre>
```

20 GetJManyRows

GetJManyColsByNames GetJManyColsByNames

Description

Returns (as a R numeric matrix) the columns with the requested column names from the matrix contained in a jmatrix binary file

Usage

```
GetJManyColsByNames(fname, extcolnames)
```

Arguments

fname String with the file name that contains the binary data.

extcolnames A numeric vector with the names of the columns to be extracted. If the binary

file has no column names, or _any_ of the column names is not present, an empty

matrix is returned.

Value

A numeric matrix with the values of elements in the requested columns

Examples

```
Rf <- matrix(runif(48),nrow=6)
rownames(Rf) <- c("A","B","C","D","E","F")
colnames(Rf) <- c("a","b","c","d","e","f","g","h")
tmpfile1=paste0(tempdir(),"/Rfullfloat.bin")
JWriteBin(Rf,tmpfile1,dtype="float",dmtype="full",comment="Full matrix of floats")
Rf[,c(1,4)]
vf<-GetJManyColsByNames(tmpfile1,c("a","d"))
vf</pre>
```

GetJManyRows

GetJManyRows

Description

Returns (as a R numeric matrix) the rows with the requested row numbers from the matrix contained in a jmatrix binary file

```
GetJManyRows(fname, extrows)
```

Arguments

fname String with the file name that contains the binary data.

extrows A numeric vector with the indexes of the rows to be extracted, in R-numbering

(from 1)

Value

A numeric matrix with the values of elements in the requested rows

Examples

```
Rf <- matrix(runif(48),nrow=6)
rownames(Rf) <- c("A","B","C","D","E","F")
colnames(Rf) <- c("a","b","c","d","e","f","g","h")
tmpfile1=paste0(tempdir(),"/Rfullfloat.bin")
JWriteBin(Rf,tmpfile1,dtype="float",dmtype="full",comment="Full matrix of floats")
Rf[c(1,4),]
vc<-GetJManyRows(tmpfile1,c(1,4))
vc</pre>
```

GetJManyRowsByNames

GetJManyRowsByNames

Description

Returns (as a R numeric matrix) the rows with the requested row names from the matrix contained in a jmatrix binary file

Usage

```
GetJManyRowsByNames(fname, extrownames)
```

Arguments

fname String with the file name that contains the binary data.

extrownames A numeric vector with the names of the rows to be extracted. If the binary file

has no row names, or _any_ of the row names is not present, an empty matrix is

returned.

Value

A numeric matrix with the values of elements in the requested rows

22 GetJNames

Examples

```
Rf <- matrix(runif(48),nrow=6)
rownames(Rf) <- c("A","B","C","D","E","F")
colnames(Rf) <- c("a","b","c","d","e","f","g","h")
tmpfile1=paste0(tempdir(),"/Rfullfloat.bin")
JWriteBin(Rf,tmpfile1,dtype="float",dmtype="full",comment="Full matrix of floats")
Rf[c("A","C"),]
vf<-GetJManyRowsByNames(tmpfile1,c("A","C"))
vf</pre>
```

GetJNames

GetJNames

Description

Returns a R list of two elements, rownames and colnames, each of them being a R StringVector with the corresponding names

Usage

```
GetJNames(fname)
```

Arguments

fname

String with the file name that contains the binary data.

Value

N["rownames","colnames"]: A list with two elements named rownames and colnames which are R StringVectors. If the binary file has no row or column names as metadata BOTH will be returned as empty vectors, even if one of them exists. If you want to extract only one, use either GetBinRowNames or GetBinColNames, as appropriate.

```
Rf <- matrix(runif(48),nrow=6)
rownames(Rf) <- c("A","B","C","D","E","F")
colnames(Rf) <- c("a","b","c","d","e","f","g","h")
tmpfile1=paste0(tempdir(),"/Rfullfloat.bin")
JWriteBin(Rf,tmpfile1,dtype="float",dmtype="full",comment="Full matrix of floats")
N<-GetJNames(tmpfile1)
N["rownames"]
N["colnames"]</pre>
```

GetJRow 23

GetJRow GetJRow

Description

Returns (as a R numeric vector) the requested row number from the matrix contained in a jmatrix binary file

Usage

```
GetJRow(fname, nrow)
```

Arguments

fname String with the file name that contains the binary data.

nrow The number of the row to be returned, in R-numbering (from 1)

Value

A numeric vector with the values of elements in the requested row

Examples

```
Rf <- matrix(runif(48),nrow=6)
rownames(Rf) <- c("A","B","C","D","E","F")
colnames(Rf) <- c("a","b","c","d","e","f","g","h")
tmpfile1=paste0(tempdir(),"/Rfullfloat.bin")
JWriteBin(Rf,tmpfile1,dtype="float",dmtype="full",comment="Full matrix of floats")
Rf[3,]
vf<-GetJRow(tmpfile1,3)
vf</pre>
```

GetJRowByName

GetJRowByName

Description

Returns (as a R numeric vector) the requested named row from the matrix contained in a jmatrix binary file

```
GetJRowByName(fname, rowname)
```

24 GetJRowNames

Arguments

fname String with the file name that contains the binary data.

rowname The name of the row to be returned. If the matrix has no row names, or the name

is not found, an empty vector is returned

Value

A numeric vector with the values of elements in the requested row

Examples

```
Rf <- matrix(runif(48),nrow=6)
rownames(Rf) <- c("A","B","C","D","E","F")
colnames(Rf) <- c("a","b","c","d","e","f","g","h")
tmpfile1=paste0(tempdir(),"/Rfullfloat.bin")
JWriteBin(Rf,tmpfile1,dtype="float",dmtype="full",comment="Full matrix of floats")
Rf["C",]
vf<-GetJRowByName(tmpfile1,"C")
vf</pre>
```

GetJRowNames

GetJRowNames

Description

Returns a R StringVector with the row names of a matrix stored in the binary format of package jmatrix, if it has them stored.

Usage

```
GetJRowNames(fname)
```

Arguments

fname

String with the file name that contains the binary data.

Value

A R StringVector with the row names, or the empty vector if the binary file has no row names as metadata.

```
Rf <- matrix(runif(48),nrow=6)
rownames(Rf) <- c("A","B","C","D","E","F")
colnames(Rf) <- c("a","b","c","d","e","f","g","h")
tmpfile1=paste0(tempdir(),"/Rfullfloat.bin")
JWriteBin(Rf,tmpfile1,dtype="float",dmtype="full",comment="Full matrix of floats")
rn<-GetJRowNames(tmpfile1)
rn</pre>
```

GetSeuratGroups 25

GetSeuratGroups

GetSeuratGroups

Description

Returns a numeric vector of integers with the numeric identifier of the group to which each cell in a Seurat object belongs to, if the cells come from different groups/samples. These numeric identifiers go from 1 to the number of groups; names of original factors are not kept.

Usage

GetSeuratGroups(q)

Arguments

q

The S4 Seurat object (for example, returned by a call to readRDS('file.rds') where the rds file was written by Seurat).

Details

If q is the Seurat object, this function assumes that

q@meta.data\$orig.ident

is the integer vector with this information. We don't know if this is assumed by all software which uses Seurat (probably, not) so this function is likely NOT to work in most cases and therefore is provided just as a convenience that can generate the parameter gr for the BuildAbundanceMatrix. But if the data you have got does not follow these conventions, please don't blame us...

Value

The numeric integer vector with as many components as cells.

- # Sorry, we cannot provide an example here, since it would need the load of the Seurat package.
- # Please, see the vignette for examples

26 GetTD

GetSubdiag

GetSubdiag

Description

Takes a symmetric matrix and returns a vector with all its elements under the main diagonal (without those at the diagonal itself) Done as an instrumental function to check the PAM in package cluster. To be removed in final version of the package.

Usage

```
GetSubdiag(fname)
```

Arguments

fname

The name of the file with the dissimilarity matrix in jmatrix binary format.

Value

The vector with the values under the main diagonal, sorted by columns (i.e.: m(2,1) ... m(n,1), m(3,2)...m(n,2),..., m(n-1,n))

Examples

```
Rns <- matrix(runif(49),nrow=7)
Rsym <- 0.5*(Rns+t(Rns))
rownames(Rsym) <- c("A","B","C","D","E","F","G")
colnames(Rsym) <- c("a","b","c","d","e","f","g")
tmpfile1=paste0(tempdir(),"/Rsymfloat.bin")
JWriteBin(Rsym,tmpfile1,dtype="float",dmtype="symmetric")
d<-GetSubdiag(tmpfile1)
Rsym
d</pre>
```

GetTD

GetTD

Description

Function that takes a PAM classification (as returned by ApplyPAM) and the dissimilarity matrix and returns the value of the TD function (sum of dissimilarities between each point and its closest medoid, divided by the number of points). This function is mainly for debugging/internal use.

```
GetTD(L, dissim_file)
```

JMatInfo 27

Arguments

A list of two numeric vectors, L["med","clasif"], as returned by ApplyPAM (please, consult the help of ApplyPAM for details)

dissim_file A string with the name of the binary file that contains the symmetric matrix of dissimilarities. Such matrix should have been generated by CalcAndWriteDis-

similarityMatrix and it is a matrix of type 'disttype' (currently defined as float).

Value

TD The value of the TD function.

Examples

```
# Synthetic problem: 10 random seeds with coordinates in [0..20]
# to which random values in [-0.1..0.1] are added
M<-matrix(0,100,500)
rownames(M)<-paste0("rn",c(1:100))</pre>
for (i in (1:10))
p<-20*runif(500)
Rf <- matrix(0.2*(runif(5000)-0.5),nrow=10)
 for (k in (1:10))
 M[10*(i-1)+k,]=p+Rf[k,]
}
}
tmpfile1=paste0(tempdir(),"/pamtest.bin")
tmpdisfile1=paste0(tempdir(),"/pamDL2.bin")
JWriteBin(M, tmpfile1, dtype="float", dmtype="full")
CalcAndWriteDissimilarityMatrix(tmpfile1,tmpdisfile1,distype="L2",restype="float",nthreads=0)
L <- ApplyPAM(tmpdisfile1,10,init_method="BUILD")</pre>
# Final value of sum of distances to closest medoid
GetTD(L,tmpdisfile1)
```

JMatInfo

JMatInfo

Description

Shows in the screen or writes to a file information about a matrix stored in the binary format of package jmatrix

```
JMatInfo(fname, fres = "")
```

JMatToCsv

Arguments

fname String with the file name that contains the binary data.

fres String with the name of the file to write the information. Default: "" (information

is written to the console)

Value

No return value, called for its side effects (writes on screen or creates a file)

Examples

```
Rf <- matrix(runif(48),nrow=6)
rownames(Rf) <- c("A","B","C","D","E","F")
colnames(Rf) <- c("a","b","c","d","e","f","g","h")
tmpfile1=paste0(tempdir(),"/Rfullfloat.bin")
JWriteBin(Rf,tmpfile1,dtype="float",dmtype="full",comment="Full matrix of floats")
JMatInfo(tmpfile1)</pre>
```

JMatToCsv

JMatToCsv

Description

Writes a binary matrix in the jmatrix package format as a .csv file. This is mainly for checking/inspection and to load the data from R as read.table, if the memory of having all data as doubles allows doing such thing.

Usage

```
JMatToCsv(ifile, csvfile, csep = ",", withquotes = FALSE)
```

Arguments

ifile	String with the file name that contains the binary data.
csvfile	String with the file name that will contain the data as csv.
csep	Character used as separator. Default: , (comma)
withquotes	boolean to mark if row and column names in the .csv file must be written surrounded by doble quotes. Default: FALSE

Value

No return value, called for side effects (creates a file)

JWriteBin 29

Examples

```
Rf <- matrix(runif(48),nrow=6)
rownames(Rf) <- c("A","B","C","D","E","F")
colnames(Rf) <- c("a","b","c","d","e","f","g","h")
tmpfile1=paste0(tempdir(),"/Rfullfloat.bin")
tmpcsvfile1=paste0(tempdir(),"/Rfullfloat.csv")
JWriteBin(Rf,tmpfile1,dtype="float",dmtype="full",comment="Full matrix of floats")
JMatToCsv(tmpfile1,tmpcsvfile1)</pre>
```

JWriteBin

Description

Writes a R matrix to a disk file as a binary matrix in the jmatrix format

Usage

```
JWriteBin(M, fname, dtype = "float", dmtype = "full", comment = "")
```

Arguments

М	The R matrix to be written
fname	The name of the file to write
dtype	The data type of the matrix to be written: one of the strings 'short', 'int', 'long', 'float' or 'double'. Default: 'float'
dmtype	The matrix type: one of the strings 'full', 'sparse' or 'symmetric'. Default: 'full'
comment	A optional string with the comment to be added as metadata. Default: "" (empty

string, no added comment)

Details

Use this function cautiously. Differently to the functions to get one or more rows or columns from the binary file, which book only the memory strictly needed for the vector/matrix and do not load all the binary file in memory, this function books the full matrix in the requested data type and writes it later so with very big matrices you might run out of memory.

Type 'int' is really long int (8-bytes in most modern machines) so using 'int' or 'long' is equivalent. Type is coerced from double (the internal type of R matrices) to the requested type, which may provoke a loose of precision.

If M is a named-R matrix, row and column names are written as metadata, too.

Also, if you write as symmetric a matrix which is not such, only the lower-diagonal part will be written. The rest of the data will be lost. In this case, if the matrix has row and column names, only row names are written.

Value

No return value, called for side effects (creates a file)

30 NumSilToClusterSil

Examples

```
Rf <- matrix(runif(48),nrow=6)
rownames(Rf) <- c("A","B","C","D","E","F")
colnames(Rf) <- c("a","b","c","d","e","f","g","h")
tmpfile1=paste0(tempdir(),"/Rfullfloat.bin")
JWriteBin(Rf,tmpfile1,dtype="float",dmtype="full",comment="Full matrix of floats")</pre>
```

NumSilToClusterSil

NumSilToClusterSil

Description

Takes a silhouette in the form of a Numeric Vector, as returned by CalculateSilhouette, and returns it as a numeric matrix appropriate to be plotted by the package 'cluster'

Usage

```
NumSilToClusterSil(cl, s)
```

Arguments

cl The array of classification with the number of the class to which each point be-

longs to. This number must be in 1..number_of_classes.

This function takes something like the L\$clasif array which is the second element of the list natural by Apply PAM

ment of the list returned by ApplyPAM

s The numeric value of the silhouette for each point, with points in the same order

as they appear in cl.

This is the vector returned by after a call to CalculateSilhouette with the same

value of parameter cl.

Value

sp A silhouette in the format of the cluster package which is a NumericMatrix of as many rows as points and three columns: cluster, neighbor and sil_width.

Its structure and dimension names are as in package 'cluster', which allows to use it with the silhouette plotting functions of such package

This means you can do library(cluster) followed by plot(NumSilToClusterSil(cl,s)) to get a beatiful plot.

```
# Synthetic problem: 10 random seeds with coordinates in [0..20]
# to which random values in [-0.1..0.1] are added
M<-matrix(0,100,500)
rownames(M)<-paste0("rn",c(1:100))
for (i in (1:10))
{
    p<-20*runif(500)</pre>
```

ScellpamSetDebug 31

ScellpamSetDebug

ScellpamSetDebug

Description

Sets debugging in scellpam package to ON (with TRUE) or OFF (with FALSE) for several parts of it.

On package load the default status is OFF.

Setting debugging of any part to ON shows a message. Setting to OFF does not show anything (since debugging is OFF...)

Usage

```
ScellpamSetDebug(deb = TRUE, debparpam = FALSE, debjmat = FALSE)
```

Arguments

deb boolean, TRUE to generate debug messages for the scellpam (biological part) of

this package and FALSE to turn them off. Default: true

debparpam boolean, TRUE to generate debug messages for the parallel PAM part inside this

package and FALSE to turn them off. Default: false

deb jmat boolean, TRUE to generate debug messages for the jmatrix part inside this pack-

age and FALSE to turn them off. Default: false

Value

No return value, called for side effects (modification of internal variables)

```
ScellpamSetDebug(TRUE, debparpam=FALSE, debjmat=FALSE)
ScellpamSetDebug(TRUE, debparpam=TRUE, debjmat=FALSE)
ScellpamSetDebug(TRUE, debparpam=TRUE, debjmat=TRUE)
```

32 SceToJMat

SceToJMat	SceToJMat	

Description

Gets a numeric matrix of counts and writes it to a disk file in the jmatrix binary format. To use this function you will have to extract yourself the matrix of counts (and may be the vectors of row names and column names) from the sce or other object type. Plase, see the Details section

Usage

```
SceToJMat(
   M,
   fname,
   rownames = NULL,
   colnames = NULL,
   mtype = "sparse",
   ctype = "raw",
   valuetype = "float",
   transpose = FALSE,
   comment = ""
)
```

Arguments

М	The numeric matrix (extracted from the sce object as counts(theobject) or otherwise directly from the sce object).
fname	A string with the name of the binary output file
rownames	The vector of strings with the row names (extracted from the sce object, or set by the user). Default: empty vector (column names will be extracted from the matrix dimnames, if present)
colnames	The vector of strings with the column names (extracted from the sce object, or set by the user). Default: empty vector (row names will be extracted from the matrix dimnames, if present)
mtype	A string to indicate the matrix type: 'full' or 'sparse'. Default: 'sparse'
ctype	The string 'raw' or 'log1' to write raw counts or log(counts+1), or the normalized versions, 'rawn' and 'log1n', which normalize ALWAYS BY COLUMNS (before transposition, if requested to transpose). Default: raw
valuetype	The data type to store the matrix. It must be one of the strings 'uint32', 'float' or 'double'. Default: float
transpose	Boolean to indicate if the matrix should be transposed before writing. See Details for a comment about this. Default: FALSE
comment	A comment to be stored with the matrix. Default: "" (no comment)

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Details

The package BiocGenerics offers a facility to get the counts matrix, function counts, so usually you may load this packages and use counts(your_sce_object) as first argument. But sometimes not, and for example in the DuoClustering, you have

M<-your object@assays\$data@listData\$counts to extract the counts matrix

but in splatter you would have

M<-your_object@assays@data@listData\$counts (which is not exactly the same...)

The message, unfortunately, is: extract the data inspecting the internal structure of the object in the package that provided the data you are using.

We assume, nevertheless, that if the matrix is M,

attr(M,"dim")[1] is the number of rows (genes)

attr(M,"dim")[2] is the number of columns (cells)

attr(M,"dimnames")[1] is the vector of row names (names of genes)

attr(M, "dimnames")[2] is the vector of column names (names of cells)

But if the matrix has not row or column names, or even if it has but you want to overwrite them, you can pass a value for parameter rownames or colnames that will be honored. If you do not pass one or both the function will try to get them from the matrix attributes, as stated before. If they do not exist as attributes in the matrix, they will be left empty.

The parameter transpose has the default value of FALSE. But don't forget to set it to TRUE if you want the cells (which in single cell common practice are by columns) to be written by rows. This will be needed later to calculate the dissimilarity matrix, if this is the next step of your workflow. See help of CalcAndWriteDissimilarityMatrix

Value

No return value, called for side effects (creates a file)

- # Sorry, we cannot provide an example here, since it would need the load of the splatter package.
- # Please, see the vignette for examples

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