

Package ‘scellpam’

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Type Package

Title Applying Partitioning Around Medoids to Single Cell Data with High Number of Cells

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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 'parallel-pam' 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)

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ApplyPAM

*ApplyPAM***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.

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 CalcAndWriteDissimilarityMatrix and it must be a symmetric matrix.
k	A positive 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` 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 number 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$med` (also from 1). This means that if `L$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 (row names) the cell names, the returned vector is a 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))
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")
# 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$med)
n[L$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 of individuals of group *c* which the classifier has identified as belonging to cluster *r*

Usage

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

Arguments

<code>clasif</code>	The vector with the number of the cluster each cell belongs to. Usually obtained as <code>L\$clasif</code> , being <code>L</code> the object returned by <code>ApplyPAM</code> . It MUST be a vector of integers with as many components as cells and values in <code>(1..number_of_clusters)</code> . Obviously, it can be a named vector but the group names are not used.
<code>gr</code>	A numeric vector with the group (of those designed for the assay) to which each cell belongs to. Normally obtained with <code>GetSeuratGroups</code> 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 <code>(1..number_of_groups)</code> . Obviously, it can be a named vector but the cell names are not used.
<code>expgroups</code>	The expected number of groups. If it is left to its default value (which is 0) the number of groups is inferred from parameter <code>grname</code> 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

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').

Usage

```
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: 'L1', 'L2', 'Pearson', 'Cos' or 'WEuc'. Respectively: L1 (Manhattan), L2 (Euclidean), Pearson (Pearson dissimilarity), Cos (cosine distance), WEuc (weighed Euclidean, with inverse-stdevs as weights). Default: 'L2'.
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 dissimilarity 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 positive 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 is 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 is 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)

Examples

```
Rf <- matrix(runif(50000),nrow=100)
tmpfile1=paste0(tempdir(),"Rfullfloat.bin")
JWriteBin(Rf,tmpfile1,dtype="float",dmtpe="full",
          comment="Full matrix of floats, 100 rows, 500 columns")
JMatInfo(tmpfile1)
tmpdisfile1=paste0(tempdir(),"RfullfloatDis.bin")
# Distance file calculated from the matrix stored as full
CalcAndWriteDissimilarityMatrix(tmpfile1,tmpdisfile1,distype="L2",
                                restype="float",comment="L2 distance matrix from full",nthreads=0)
JMatInfo(tmpdisfile1)
tmpfile2=paste0(tempdir(),"Rsparsefloat.bin")
JWriteBin(Rf,tmpfile2,dtype="float",dmtpe="sparse",
          comment="Sparse matrix of floats, 100 rows, 500 columns")
JMatInfo(tmpfile2)
# Distance file calculated from the matrix stored as sparse
tmpdisfile2=paste0(tempdir(),"RsparsefloatDis.bin")
CalcAndWriteDissimilarityMatrix(tmpfile2,tmpdisfile2,distype="L2",
                                restype="float",comment="L2 distance matrix from sparse",nthreads=0)
JMatInfo(tmpdisfile2)
# Read both versions
Dfu<-GetJManyRows(tmpdisfile1,c(1:nrow(Rf)))
Dsp<-GetJManyRows(tmpdisfile2,c(1:nrow(Rf)))
# and compare them
max(Dfu-Dsp)
```

CalculateSilhouette *CalculateSilhouette*

Description

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

Usage

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

Arguments

<code>cl</code>	The array of classification with the number of the class to which each point belongs to. This number must be in $1..number_of_classes$. This function takes something like the <code>L\$clasif</code> array which is the second element of the list returned by <code>ApplyPAM</code>
<code>fdist</code>	The binary file containing the symmetric matrix with the dissimilarities between cells (usually, generated by a call to <code>CalcAndWriteDissimilarityMatrix</code>)
<code>nthreads</code>	The number of used threads for parallel calculation. -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 number 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 are in `cl`.
If `cl` is a named vector `sil` will be a named vector, too, with the same names.

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))
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")
sil <- CalculateSilhouette(L$clasif,tmpdisfile1)
# Histogram of the silhouette. In this synthetic problem, almost 1 for all points
hist(sil)
```

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).

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.

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))
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",dmtpe="full")
tmpdisfile1=paste0(tempdir(),"/pamDL2.bin")
CalcAndWriteDissimilarityMatrix(tmpfile1,tmpdisfile1,distype="L2",restype="float",nthreads=0)
L <- ApplyPAM(tmpdisfile1,10,init_method="BUILD")
df <- ClassifAsDataFrame(L,tmpdisfile1)
df
# Identification of medoids:
which(df[,3]==0)
# Verification they are the same as in L (in different order)
```

L\$med

ClosestCases

ClosestCases

Description

Gets a matrix of size $n \times p$ where each file represents an individual (gene, cell,..) and each column its characteristics (counts,...) stored in a file in jmatrix format and returns a matrix of $n \times p$ with contains, for each individual the indices of the q individuals closest to it. To do so, the Pearson correlation coefficient is calculated between each row. Then, closeness can be measured directly, as the q values with higher value, but also in a more sophisticated way using the p-values to consider null correlations.

Usage

```
ClosestCases(datafile, q = 5L, method = "trivial", dvalue = 0, nthreads = 0L)
```

Arguments

datafile	A string with the name of the file containing the individuals/characteristics in jmatrix format.
q	The name of closest related individuals to be returned. Default: 5
method	The method to be applied to choose the closest values. It must be one of these strings: 'trivial', 'absvalue', 'FDR'.
dvalue	The value of the absolute value of the Pearson coefficient or of the False Discovery Rate (FDR), depending on the value of the 'method' parameter
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 positive number > 1: use that number of threads. You can use even more than cores, but this is discouraged and raises a warning. Default: 0.

Value

A $n \times q$ matrix with the indices (in R notation, starting at 1) of the individuals closest to the individual i at i -th row Index will be 0 in some cases if less than q individuals are found to be close according to the 'absvalue' or 'FDR' criteria

Examples

```
# To be done
```

 CsvToJMat

CsvToJMat

Description

Gets a csv/tsv 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 row name.

The fields are supposed to be separated by one occurrence of a character-field separator (usually, comma or tab) .tsv files can be read with this function, too, setting the csep argument to '\t'

Usage

```
CsvToJMat(
  ifname,
  ofname,
  mtype = "sparse",
  csep = ",",
  ctype = "raw",
  valuetype = "float",
  transpose = FALSE,
  comment = ""
)
```

Arguments

ifname	A string with the name of the .csv/.tsv text file.
ofname	A string with the name of the binary output file.
mtype	A string to indicate the matrix type: 'full', 'sparse' or 'symmetric'. Default: 'sparse'
csep	The character used as separator in the .csv file. Default: ',' (comma) (Set to '\t' for .tsv)
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). 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 Details 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`

Special note for loading symmetric matrices:

If you use this function to load what you expect to be a symmetric matrix from a `.csv` file, remember that the input table **MUST** be square, but only the lower-diagonal matrix will be stored, including the main diagonal. The rest of the input table is completely ignored, except to check that there are values in it. It is not checked if the table really represents a symmetric matrix or not.

Furthermore, symmetric matrices can only be loaded in raw mode, i.e.: no normalization is allowed, and they cannot be transposed.

Value

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

Examples

```
# Since we have no a .csv file to test, we will generate one with another function 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")
tmppcsvfile1=paste0(tempdir(),"Rfullfloat.csv")
JWriteBin(Rf,tmpfile1,dtype="float",dmtpe="full",comment="Full matrix of floats")
JMatToCsv(tmpfile1,tmppcsvfile1)
CsvToJMat(tmppcsvfile1,tmpfile2)
# It can be checked that files Rfullfloat.bin and Rfullfloat2.bin contain the same data
# (even they differ in the comment, which has been eliminated when converting to csv)
```

dgCMatToJMat

dgCMatToJMat

Description

Gets a `dgCMatrix` object (sparse matrix of the ‘Matrix’ package) and writes to a disk file the binary matrix of counts contained in it in the `jmatrix` binary format. Please, 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 'Matrix' package 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

```

`ExtractAndWriteDissimilarityMatrix`*ExtractAndWriteDissimilarityMatrix*

Description

Writes a binary symmetric matrix with some of the dissimilarities stored in a binary matrix in the scellpam package format.

The purpose of this function is to get the dissimilarity matrix between some selected individuals of a larger set whose dissimilarity matrix has been calculated before without calculating explicitly the dissimilarities again. The extracted matrix has the same data type as the original and of course is a symmetric matrix, too. A comment can be added to the original matrix comment or set, if there was no previous comment.

Usage

```
ExtractAndWriteDissimilarityMatrix(ifname, ofname, select, comment = "")
```

Arguments

<code>ifname</code>	A string with the name of the file containing the original dissimilarity matrix in jmatrix format
<code>ofname</code>	A string with the name of the file to contain the symmetric dissimilarity matrix between the selected rows.
<code>select</code>	A boolean array with length equal to the size of the original matrix indicating (with true) which rows/columns must be extracted.
<code>comment</code>	Comment to be attached to the dissimilarity matrix, added to the comment of the original one. Default: "" (no comment)

Value

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

Examples

```
# TO BE DONE
```

 FilterBySilhouetteQuantile

FilterBySilhouetteQuantile

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 silhouette 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 silhouette 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.
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.
q	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. Successive 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$med` is a modification of the corresponding first element of the passed `L` parameter.
`Lr$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

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))
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",dmtpe="full")
tmpdisfile1=paste0(tempdir(),"/pamDl2.bin")
CalcAndWriteDissimilarityMatrix(tmpfile1,tmpdisfile1,distype="L2",restype="float",nthreads=0)
L <- ApplyPAM(tmpdisfile1,10,init_method="BUILD")
# Which are the medoids
L$med
sil <- CalculateSilhouette(L$clasif,tmpdisfile1)
tmpfiltfile1=paste0(tempdir(),"/pamtestfilt.bin")
tmpfiltdisfile1=paste0(tempdir(),"/pamDL2filt.bin")
Lf<-FilterBySilhouetteQuantile(sil,L,tmpfile1,tmpfiltfile1,tmpdisfile1,tmpfiltdisfile1,
                              q=0.4,addcom=TRUE)
# The new medoids are the same points but renumbered, since the L$clasif array has less points
Lf$med
```

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 silhouette 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 silhouette 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.
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.
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. Successive 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 corresponding 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

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))
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",dmtpe="full")
tmpdisfile1=paste0(tempdir(),"/pamDl2.bin")
CalcAndWriteDissimilarityMatrix(tmpfile1,tmpdisfile1,distype="L2",restype="float",nthreads=0)
L <- ApplyPAM(tmpdisfile1,10,init_method="BUILD")
# Which are the medoids
L$med
sil <- CalculateSilhouette(L$clasif,tmpdisfile1)
tmpfiltfile1=paste0(tempdir(),"/pamtestfilt.bin")
tmpfiltdisfile1=paste0(tempdir(),"/pamDL2filt.bin")
Lf<-FilterBySilhouetteThreshold(sil,L,tmpfile1,tmpfiltfile1,tmpdisfile1,tmpfiltdisfile1,
                               thres=0.4,addcom=TRUE)
# The new medoids are the same points but renumbered, since the L$clasif array has less points
Lf$med
```

FilterJMatByName	<i>FilterJMatByName</i>
------------------	-------------------------

Description

Takes a jmatrix binary file containing a table with rows and columns and filters it by name, eliminating the rows or columns whose names are not in certain list

Usage

```
FilterJMatByName(fname, Gn, filename, 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 rows or columns that must remain. All others will be filtered out
filename	A string with the file name of the filtered table
namesat	The string "rows" or "cols" indicating if the searched names are in the rows or in the columns of the original table. Default: "rows"

Details

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

The row or column names whose names are not found obviously cannot remain, and the program raises a warning indicating for which row/column 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 row or by column name, with appropriate usage of parameter namesat

Value

No return value, called for side effects (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")
tmpfile2=paste0(tempdir(),"Rfullfloatrowfilt.bin")
tmpfile3=paste0(tempdir(),"Rfullfloatrowcolfilt.bin")
tmppsvfile1=paste0(tempdir(),"Rfullfloat.csv")
tmppsvfile3=paste0(tempdir(),"Rfullfloatrowcolfilt.csv")
JWriteBin(Rf,tmpfile1,dtype="float",dmtpe="full",comment="Full matrix of floats")
# Let's keep only rows A, C and E
```

```

FilterJMatByName(tmpfile1,c("A","C","E"),tmpfile2,namesat="rows")
# 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

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",dmtpe="full",comment="Full matrix of floats")
Rf[,3]
vf<-GetJCol(tmpfile1,3)
vf

```

GetJColByName	<i>GetJColByName</i>
---------------	----------------------

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",dmtpe="full",comment="Full matrix of floats")
Rf[,"c"]
vf<-GetJColByName(tmpfile1,"c")
vf
```

GetJColNames	<i>GetJColNames</i>
--------------	---------------------

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.

Usage

```
GetJColNames(fname)
```

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 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",dmtpe="full",comment="Full matrix of floats")
cn<-GetJColNames(tmpfile1)
cn
```

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

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",dmtpe="full",comment="Full matrix of floats")
vc<-GetJManyCols(tmpfile1,c(1,4))
vc
```

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 vector of RStrings 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",dmtpe="full",comment="Full matrix of floats")
Rf[,c(1,4)]
vf<-GetJManyColsByNames(tmpfile1,c("a","d"))
vf
```

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

Usage

```
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",dmtpe="full",comment="Full matrix of floats")
Rf[c(1,4),]
vc<-GetJManyRows(tmpfile1,c(1,4))
vc
```

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 vector of RStrings with the names of the rows to be extracted. If the binary file has no row names, or <i>_any_</i> 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

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",dmtpe="full",comment="Full matrix of floats")
Rf[c("A","C"),]
vf<-GetJManyRowsByNames(tmpfile1,c("A","C"))
vf
```

 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 GetJRowNames or GetJColNames, as appropriate.

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",dmtpe="full",comment="Full matrix of floats")
N<-GetJNames(tmpfile1)
N["rownames"]
N["colnames"]
```

GetJRow	<i>GetJRow</i>
---------	----------------

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",dmtpe="full",comment="Full matrix of floats")
Rf[3,]
vf<-GetJRow(tmpfile1,3)
vf
```

GetJRowByName	<i>GetJRowByName</i>
---------------	----------------------

Description

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

Usage

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

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",dmtpe="full",comment="Full matrix of floats")
Rf["C",]
vf<-GetJRowByName(tmpfile1,"C")
vf
```

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.

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",dmtpe="full",comment="Full matrix of floats")
rn<-GetJRowNames(tmpfile1)
rn
```

GetSeuratGroups	<i>GetSeuratGroups</i>
-----------------	------------------------

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.

Examples

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

GetSubdiag	<i>GetSubdiag</i>
------------	-------------------

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.: $m(2,1) \dots m(n,1)$, $m(3,2) \dots m(n,2)$, ..., $m(n-1,n)$)

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",dmtpe="symmetric")
d<-GetSubdiag(tmpfile1)
Rsym
d
```

GetTD	<i>GetTD</i>
-------	--------------

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.

Usage

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

Arguments

- L** 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 CalcAndWriteDissimilarityMatrix.

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))
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",dmtpe="full")
CalcAndWriteDissimilarityMatrix(tmpfile1,tmpdisfile1,distype="L2",restype="float",nthreads=0)
L <- ApplyPAM(tmpdisfile1,10,init_method="BUILD")
# 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

Usage

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

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",dmtpe="full",comment="Full matrix of floats")
JMatInfo(tmpfile1)
```

JMatInfoList

JMatInfoList

Description

Returns a list with information about a matrix stored in the binary format of package jmatrix

Usage

```
JMatInfoList(fname)
```

Arguments

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

Value

A list with the following keys:

- `mattpe` - String with one of the values "full", "sparse", "symmetric" or "unknown"
- `datatype` - String with one of the values "uchar", "char", "ushort", "short", "uint", "int", "ulong", "long", "float", "double", "ldouble" or "unknown"
- `endian` - String with one of the values "little", "big"
- `nrows` - Integer, the number of rows
- `ncols` - Integer, the number of cols
- `comment` - String with the comment, if stored, or the empty string otherwise

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")
L <- JMatInfoList(tmpfile1)
cat(sep="","Matrix in file ",tmpfile1," is ",L$matttype," has elements of type ")
cat(sep=" ",L$datatype," stored in ",L$endian," endian, its size is ",L$nrows," x ",L$ncols,"\n")
if (L$comment=="") { cat("Attached comment:\n",L$comment,"\n") }
```

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.csv, 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 double quotes. Default: FALSE

Details

The numbers are written to text with as many decimal places as allowed by its data type (internally obtained with `std::numeric_limits<type>::max_digits10`)

NOTE ON READING FROM R: to read the .csv files exported by this function you MUST use the R function `read.csv` (not `read.table`) AND set its argument `row.names` to 1, since we always write a first column with the row names, even if the binary matrix does not store them; in this case they are simply "1","2",...

Value

No return value, called for side effects (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")
tmpcsvfile1=paste0(tempdir(),"Rfullfloat.csv")
JWriteBin(Rf,tmpfile1,dtype="float",dmtpe="full",comment="Full matrix of floats")
JMatToCsv(tmpfile1,tmpcsvfile1)
```

JWriteBin

JWriteBin

Description

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

Usage

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

Arguments

M	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'
dmtpe	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)

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",dmtpe="full",comment="Full matrix of floats")
```

NumSilToClusterSil *NumSilToClusterSil*

Description

Takes a silhouette in the form of a NumericVector, 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 belongs 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 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 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 with 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 beautiful plot.

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))
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",dmtpe="full")
tmpdisfile1=paste0(tempdir(),"/pamDL2.bin")
CalcAndWriteDissimilarityMatrix(tmpfile1,tmpdisfile1,distype="L2",restype="float",nthreads=0)
L <- ApplyPAM(tmpdisfile1,10,init_method="BUILD")
sil <- CalculateSilhouette(L$clasif,tmpdisfile1)
sp <- NumSilToClusterSil(L$clasif,sil)
library(cluster)
plot(sp)
```

ScellpamGetDebug

ScellpamGetDebug

Description

Obtains the current state of the debugging parameter. To be used by R functions which want to adjust their messages according to the general debugging settings.

Usage

```
ScellpamGetDebug()
```

Value

A list with the following keys:

- deb - Boolean with the current debugging value of the scellpam (biological part) of this package
- debparpam - Boolean with the current debugging value of the parallel PAM part inside this package
- debjmat - Boolean with the current debugging value of the jmatrix part inside this package

Examples

```
d<-ScellpamGetDebug()
```

ScellpamSetDebug	<i>ScellpamSetDebug</i>
------------------	-------------------------

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
debjmat	boolean, TRUE to generate debug messages for the jmatrix part inside this package and FALSE to turn them off. Default: false

Value

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

Examples

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

SceToJMat	<i>SceToJMat</i>
-----------	------------------

Description

Gets a numeric matrix of counts in the single cell experiment (sce) format 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

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

Arguments

M	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)

Details

The package BiocGenerics offers a facility to get the counts matrix, the function 'counts', so usually you may load this package 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 columns 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)

Examples

```
# 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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