Package ‘M3C’

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Title Monte Carlo Reference-based Consensus Clustering
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Description M3C is a consensus clustering algorithm that uses a Monte Carlo simulation to eliminate overestimation of K and can reject the null hypothesis K=1.
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clusterm: A cluster simulator for testing clustering algorithms

Description

clusterm: A cluster simulator for testing clustering algorithms

Usage

clusterm(n, n2, r, K, alpha, wobble, redp = NULL, print = FALSE, seed = NULL)

Arguments

n Numerical value: The number of samples, it must be square rootable
n2 Numerical value: The number of features
r Numerical value: The radius to define the initial circle (use approx n/100)
K Numerical value: How many clusters to simulate
alpha Numerical value: How far to pull apart the clusters
wobble Numerical value: The degree of noise to add to the sample coordinates
redp Numerical value: The fraction of samples to remove from one cluster
print Logical flag: whether to print the PCA into current directory
seed Numerical value: fixes the seed if you want to repeat results

Value

A list: containing 1) matrix with simulated data in it

Examples

res <- clusterm(225, 900, 8, 4, 0.75, 0.025, redp = NULL, seed=123)
### GBM clinical annotation data

**Description**

This is the clinical annotation data from the GBM dataset, it contains the class of the tumour which is one of: classical, mesenchymal, neural, proneural. It is a data frame with 2 columns and 50 rows.

**Author(s)**

Chris John &lt;chris.r.john86@gmail.com&gt;

**References**


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### featurefilter: A function for filtering features

**Description**

This function is to filter features based on variance. Depending on the data different metrics will be more appropriate, simple variance is included if variance does not tend to increase with the mean. There is also the median absolute deviation which is a more robust metric than variance, this is preferable. The coefficient of variation (A) or its second order derivative (A2) (Kvalseth, 2017) are also included which standardise the standard deviation with respect to the mean. It is best to manually examine the mean-variance relationship of the data, for example, using the results from this function together with the qplot function from ggplot2.

**Usage**

\[
\text{featurefilter}(\text{mydata, percentile = 10, method = "MAD", topN = 20})
\]

**Arguments**

- **mydata**: Data frame: should have samples as columns and rows as features
- **percentile**: Numerical value: the top X percent most variable features should be kept
- **method**: Character vector: variance (var), coefficient of variation (A), second order A (A2), median absolute deviation (MAD)
- **topN**: Numerical value: the number of most variable features to display
**Value**

A list, containing: 1) filtered data 2) statistics for each feature order according to the defined filtering metric

**References**


**Examples**

```r
filtered <- featurefilter(mydata, percentile=10)
```

---

**M3C: Monte Carlo Reference-based Consensus Clustering**

**Description**

This is the M3C core function, which is a reference-based consensus clustering algorithm. The basic idea is to use a multi-core enabled Monte Carlo simulation to drive the creation of a null distribution of stability scores. The Monte Carlo simulations maintains the feature correlation structure of the input data. Then the null distribution is used to compare the reference scores with the real scores and an empirical p value is calculated for every value of K to test the null hypothesis K=1. We derive the Relative Cluster Stability Index (RCSI) as a metric for selecting K, which is based on a comparison against the reference mean. A fast alternative is also included that includes a penalty term to prevent overestimation of K, we call regularised consensus clustering.

**Usage**

```r
M3C(mydata, cores = 1, iters = 25, maxK = 10, pItem = 0.8,
    des = NULL, ref_method = c("reverse-pca", "chol"), repsref = 100,
    repsreal = 100, clusteralg = c("pam", "km", "spectral", "hc"),
    pacx1 = 0.1, pacx2 = 0.9, seed = 123, objective = "entropy",
    removeplots = FALSE, silent = FALSE, fsize = 18, method = 1,
    lambdadefault = 0.1, tunelambda = TRUE, lseq = seq(0.02, 0.1, by = 0.02), lthick = 2, dotsize = 3)
```

**Arguments**

- **mydata**: Data frame or matrix: Contains the data, with samples as columns and rows as features
- **cores**: Numerical value: how many cores to split the monte carlo simulation over
- **iters**: Numerical value: how many Monte Carlo iterations to perform (default: 25, recommended: 5-100)
- **maxK**: Numerical value: the maximum number of clusters to test for, K (default: 10)
- **pItem**: Numerical value: the fraction of points to resample each iteration (default: 0.8)
**M3C**

- **des**: Data frame: contains annotation data for the input data for automatic reordering
- **ref_method**: Character string: refers to which reference method to use
- **repsref**: Numerical value: how many resampling reps to use for reference (default: 100, recommended: 100-250)
- **repsreal**: Numerical value: how many resampling reps to use for real data (default: 100, recommended: 100-250)
- **clusteralg**: String: dictates which inner clustering algorithm to use (default: PAM)
- **pacx1**: Numerical value: The 1st x co-ordinate for calculating the pac score from the CDF (default: 0.1)
- **pacx2**: Numerical value: The 2nd x co-ordinate for calculating the pac score from the CDF (default: 0.9)
- **seed**: Numerical value: specifies seed, set to NULL for different results each time
- **objective**: Character string: whether to use 'PAC' or 'entropy' objective function (default = entropy)
- **removeplots**: Logical flag: whether to remove all plots from view
- **silent**: Logical flag: whether to remove messages or not
- **fsize**: Numerical value: determines the font size of the ggplot2 plots
- **method**: Numerical value: 1 refers to the Monte Carlo simulation method, 2 to regularised consensus clustering
- **lambdadefault**: Numerical value: if not tuning fixes the default (default: 0.1)
- **tunelambda**: Logical flag: whether to tune lambda or not
- **lseq**: Numerical vector: vector of lambda values to tune over (default = seq(0.05,0.1,by=0.01))
- **lthick**: Numerical value: determines the line thickness of the ggplot2 plot
- **dotsize**: Numerical value: determines the dotsize of the ggplot2 plot

**Value**

A list, containing: 1) the stability results and 2) all the output data (another list) 3) reference stability scores (see vignette for more details on how to easily access)

**Examples**

```r
res <- M3C(mydata)
```
mydata  

GBM expression data

Description

This is the expression data from the GBM dataset. It is a data frame with 50 columns and 1740 rows.

Author(s)

Chris John <chris.r.john86@gmail.com>

References


pca  

pca: A principal component analysis function

Description

This is a flexible PCA function that can be run on a standard data frame. It is a wrapper for prcomp/ggplot2 code and can be customised with different colours and font sizes and more.

Usage

```
pca(mydata, printres = FALSE, labels = FALSE, text = FALSE, axistextsize = 18, legendtextsize = 18, dotsize = 5, textlabelsize = 4, legendtitle = "Group", controlscale = FALSE, scale = 1, low = "grey", high = "red", colvec = c("skyblue", "gold", "violet", "darkorchid", "slateblue", "forestgreen", "violetred", "orange", "midnightblue", "grey31", "black"), printheight = 20, printwidth = 22, pcx = 1, pcy = 2, scaler = FALSE)
```

Arguments

- **mydata**  
  Data frame or matrix: if dataframe/matrix should have samples as columns and rows as features
- **printres**  
  Logical flag: whether to print the PCA into current directory
- **labels**  
  Character vector: if we want to just label with gender for example
- **text**  
  Character vector: if we wanted to label the samples with text IDs to look for outliers
tsne

DESCRIPTION

This is a flexible t-SNE function that can be run on a standard data frame. It is a wrapper for Rtsne/ggplot2 code and can be customised with different colours and font sizes and more.

USAGE

```
    tsne(mydata, labels = FALSE, perplex = 15, printres = FALSE,
         seed = FALSE, axistextsize = 18, legendtextsize = 18,
         dotsize = 5, textlabelsize = 4, legendtitle = "Group",
         controlscale = FALSE, scale = 1, low = "grey", high = "red",
         colvec = c("skyblue", "gold", "violet", "darkorchid", "slateblue",
                     "forestgreen", "violetred", "orange", "midnightblue", "grey31", "black"),
         printheight = 20, printwidth = 22, text = FALSE)
```

VALUE

A PCA plot object

EXAMPLES

```
    PCA <- pca(mydata)
```
Arguments

- **mydata**: Data frame or matrix: if dataframe/matrix should have samples as columns and rows as features
- **labels**: Character vector: if we want to just label with gender for example
- **perplex**: Numerical value: perplexity value that Rtsne uses internally
- **printres**: Logical flag: whether to print the t-SNE into current directory
- **seed**: Numerical value: optionally set the seed
- **axistextsize**: Numerical value: axis text size
- **legendtextsize**: Numerical value: legend text size
- **dotsize**: Numerical value: dot size
- **textlabelsizesize**: Numerical value: text inside plot label size
- **legendtitle**: Character vector: text legend title
- **controlscale**: Logical flag: whether to control the colour scale
- **scale**: Numerical value: 1=spectral palette, 2=manual low and high palette, 3=categorical labels
- **low**: Character vector: continuous scale low colour
- **high**: Character vector: continuous scale high colour
- **colvec**: Character vector: a series of colours in vector for categorical labels, e.g. c("sky blue", "gold")
- **printheight**: Numerical value: png height
- **printwidth**: Numerical value: png width
- **text**: Character vector: if we wanted to label the samples with text IDs to look for outliers

Value

A t-SNE plot object

Examples

```r
TSNE <- tsne(mydata, perplex=15)
```

umap: A umap function

Description

This is a flexible umap function that can be run on a standard data frame. It is a wrapper for umap/ggplot2 code and can be customised with different colours and font sizes and more.
Usage

`umap(mydata, labels = FALSE, printres = FALSE, seed = FALSE,`  
`axistextsize = 18, legendtextsize = 18, dotsize = 5,`  
`textlabelsiz e = 4, legendtitle = "Group", controlscale = FALSE,`  
`scale = 1, low = "grey", high = "red", colvec = c("skyblue", "gold", "violet", "darkorchid", "slateblue", "forestgreen", "violetred", "orange", "midnightblue", "grey31", "black"), printheight = 20,`  
`printwidth = 22, text = FALSE)`

Arguments

`mydata` Data frame or matrix: if dataframe/matrix should have samples as columns and rows as features
`labels` Character vector: if we want to just label with gender for example
`printres` Logical flag: whether to print the UMAP into current directory
`seed` Numerical value: optionally set the seed
`axistextsize` Numerical value: axis text size
`legendtextsize` Numerical value: legend text size
`dotsize` Numerical value: dot size
`textlabelsiz e` Numerical value: text inside plot label size
`legendtitle` Character vector: text legend title
`controlscale` Logical flag: whether to control the colour scale
`scale` Numerical value: 1=spectral palette, 2=manual low and high palette, 3=categorical labels
`low` Character vector: continuous scale low colour
`high` Character vector: continuous scale high colour
`colvec` Character vector: a series of colours in vector for categorical labels, e.g. c("sky blue", "gold")
`printheight` Numerical value: png height
`printwidth` Numerical value: png width
`text` Character vector: if we wanted to label the samples with text IDs to look for outliers

Value

A umap plot object

Examples

`UMAP <- umap(mydata)`
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