

Package ‘bigMap’

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Type Package

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bdm.boxp	<i>Clustering statistics box-plot.</i>
----------	--

Description

Clustering statistics box-plot.

Usage

```
bdm.boxp(bdm, byVars = F, layer = 1)
```

Arguments

bdm	A <i>bdm</i> instance as generated by <code>bdm.init()</code> .
byVars	A logical value. By default (<code>byVars = FALSE</code>) box-plots are grouped by cluster. With <code>byVars = TRUE</code> box-plots are grouped by input feature.
layer	The number of a layer (1 by default).

Details

If the number of clusters is large, only the first 25 clusters will be plotted. Note that the WTT algorithm numbers the clusters based on density value at the peak cell of the cluster. Thus, the numbering of the clusters is highly correlated with their relevance in terms of partial density. Therefore, in case of more than 25 clusters, the most relevant should always be included in the plot.

Value

None.

Examples

```
bdm.example()
bdm.boxp(exMap)
bdm.boxp(exMap, byVars = TRUE)
```

bdm.cost	<i>ptSNE cost & size plot.</i>
----------	------------------------------------

Description

ptSNE cost & size plot.

Usage

```
bdm.cost(bdm, offset = 0)
```

Arguments

bdm	A <i>bdm</i> instance as generated by <code>bdm.init()</code> or a list of them to make a comparative plot.
offset	X-axis offset in number of epochs (0 by default).

Value

None.

Examples

```
bdm.example()
bdm.cost(exMap)
```

bdm.dMap	<i>Class density maps</i>
----------	---------------------------

Description

Compute the class density maps of a set of classes on the embedding grid. This function returns a fuzzy mapping of the set of classes on the grid cells. The classes can be whatever set of classes of interest and must be given as a vector of point-wise discrete labels (either numeric, string or factor).

Usage

```
bdm.dMap(bdm, threads = 2, type = "SOCK", labels = NULL, layer = 1)
```

Arguments

bdm	A <i>bdm</i> instance as generated by <code>bdm.init()</code> .
threads	The number of parallel threads (in principle only limited by hardware resources, i.e. number of cores and available memory)
type	The type of cluster: 'SOCK' (default) for intra-node parallelization, 'MPI' for inter-node parallelization (message passing interface parallel environment).
labels	A vector of point-wise covariate values or class labels. The covariate values can be of any factorizable type. By default (<code>labels=NULL</code>) the function computes the density maps based on the clustering labels (i.e. equivalent to <code>labels=bdm.labels(bdm)</code>)
layer	The number of the t-SNE layer (1 by default).

Details

`bdm.dMap()` computes the joint distribution $P(V = v_i, C = c_j)$ where $V = v_1, \dots, v_l$ is the discrete covariate and $C = c_1, \dots, c_g$ are the grid cells of the paKDE raster. That is, this function recomputes the paKDE but keeping track of the covariate (or class) label of each data-point. This results in a fuzzy distribution of the covariate (class) at each cell.

Usually, figuring out the joint distribution $P(V = v_i, C = c_j)$ entails an intensive computation. Thus `bdm.dMap()` performs the computation and stores the result in a dedicated element named *\$dMap*. Afterwards the class density maps can be visualized with the `bdm.dMap.plot()` function.

Value

A copy of the input *bdm* instance with element *\$dMap*, a matrix with a soft clustering of the grid cells.

Examples

```
# --- load example dataset
bdm.example()
## Not run:
exMap <- bdm.dMap(exMap, threads = 4)

## End(Not run)
```

bdm.dMap.plot

Class density maps plot.

Description

Class density maps plot.

Usage

```
bdm.dMap.plot(bdm, classes = NULL, join = FALSE, class.pltt = NULL,
  pakde.pltt = NULL, pakde.lvls = 16, wtt.lwd = 1, plot.peaks = T,
  labels.cex = 1, layer = 1)
```

Arguments

<code>bdm</code>	A <i>bdm</i> instance as generated by <code>bdm.init()</code> .
<code>classes</code>	A vector with a subset of class names or covariate values. Default value is <code>classes=NULL</code> . If no classes are specified (default value) all classes are plotted.
<code>join</code>	Logical value. If <code>FALSE</code> (default value), class mapping is based on the class conditional distributions. If <code>TRUE</code> , class mapping is based on the overall classes join distribution.
<code>class.pltt</code>	A palette of colours to identify the classes in the hard mapping. The length of the colour palette should be at least the number of classes plus one (the background colour being the first colour of the palette).
<code>pakde.pltt</code>	A palette of colours to indicate the levels of the class density maps. The length of the colour palette should be at least the number of levels specified in <i>pakde.lvls</i> .
<code>pakde.lvls</code>	The number of levels of the heat-map when plotting class density maps (16 by default).
<code>wtt.lwd</code>	The width of the watertrack lines (as set in <code>par()</code>).
<code>plot.peaks</code>	Logical value (<code>TRUE</code> by default). If set to <code>TRUE</code> and the up-stream step <code>bdm\$wtt()</code> is computed the peak of each cluster is depicted.
<code>labels.cex</code>	If <i>plot.peaks</i> is <code>TRUE</code> , the size of the labels of the clusters (as set in <code>par()</code>). By default <code>labels.cex=0.0</code> and the labels of the clusters are not depicted.
<code>layer</code>	The number of the layer from which the class density maps are computed (1 by default).

Details

`bdm.dMap.plot()` yields a multi-plot layout where the first plot shows the dominating value of the covariate (or dominating class) in each cell, and the rest of the plots show the density map of each covariate value (or class).

The join distribution $P(V = v_i, C = c_j)$ will be affected by the bias present in the marginal distribution of the covariate. Therefore, the join distribution $P(V = v_i, C = c_j)$ is transformed, by default, into a conditional distribution $P(c_j|V = v_i)$ (where the c_j are the grid cells of the embedding and V is the covariate (or class)). Thus, the first plot shows a hard classification of grid-cells, (cells are coloured based on the dominating value of the covariate (or dominating class), *i.e.* the v_i for which $P(c_j|V = v_i)$ is maximum), and the rest of the plots show the conditional distributions $P(C = c_j|V = v_i)$. This makes the plots of the different classes not directly comparable but the dominant areas of each class can be more easily identified.

However, the same plots can be depicted based on the join distribution by setting `join = TRUE`. This makes sense when the bias in the covariate values (or classes) is not significant. In this case the hard clustering shows the real dominance of each covariate value (or class) over the embedding

area and the density maps are comparable one to each other (although, individually, they are not real density functions as they do not add up to one).

The multi-plot layout can be limited to a subset of the values of the covariate (or subset of classes) specified in parameter `classes`.

Value

None.

Examples

```
# --- load example dataset
bdm.example()
## Not run:
exMap <- bdm.dMap(exMap, threads = 4)
bdm.dMap.plot(exMap)

## End(Not run)
```

bdm.example

Example dataset

Description

Loads an example of a mapping of a dataset.

Usage

```
bdm.example()
```

Details

A *bdm* instance is a list with elements: *\$dSet* a name identifying the dataset (`bdm.fName()` use this name to generate a default file name); *\$data* a matrix with raw data; *\$lbls* a vector of datapoint labels (in case they are known); *\$N* the dataset size; *\$is.distance* a logical value that is set to TRUE when the raw data is a distance matrix. Downstream steps of the mapping protocol will add more elements to the list.

This example is based on a small synthetic dataset with $n = 5000$ observations drawn from a 4-variate Gaussian Mixture Model (GMM) with 16 Gaussian components.

Value

An example *bdm* instance named *exMap*.

Examples

```
# --- load example dataset
bdm.example()
str(exMap)
```

bdm.fName	<i>Default bdm file name</i>
-----------	------------------------------

Description

Generates a default file name. The default file name is intended for functions `bdm.save()` and `bdm.scp()` to ease the task of working/organizing multiple runs on the same dataset.

Usage

```
bdm.fName(bdm)
```

Arguments

bdm A *bdm* instance as generated by `bdm.init()`.

Details

The file name is generated based on `bdm$dSet` and main ptSNE parameters (threads, layers, rounds, boost and perplexity). In case that `bdm.wtt()` has been performed on any of the layers, the number of clusters in the first not null layer of `bdm$wtt` is also included.

Value

A **.RData* file name based on `bdm$dSet` and main *bdm* parameters.

Examples

```
bdm.example()
str(exMap$dSet)
str(exMap$ptsne)
bdm.fName(exMap)
```

bdm.init	<i>Create bdm instance</i>
----------	----------------------------

Description

Creates a *bdm* instance.

Usage

```
bdm.init(dSet.name, dSet.data, labels = NULL, is.distance = F,
         check.duplicates = T)
```

Arguments

<code>dSet.name</code>	The name given to the input dataset. This name will be used to automatically generate a name to save the output as an <i>.Rdata</i> file.
<code>dSet.data</code>	A <i>data.frame</i> or <i>matrix</i> with raw input-data. The dataset must not have duplicated rows.
<code>labels</code>	If available, labels can be included as a separate vector of length equal to <code>nrow(dSet.data)</code> . Label values are factorized as <code>as.numeric(as.factor(labels))</code> .
<code>is.distance</code>	A logical value (<code>FALSE</code> by default). <code>TRUE</code> indicates that the raw data is indeed a distance matrix.
<code>check.duplicates</code>	If set to <code>TRUE</code> (default value) the dataset is checked for duplicated rows. Checking for duplicates in big datasets can take some time. If the dataset is known to have no duplicates disabling this option will save time.

Value

A *bdm* instance. A *bdm* instance is initially a list with a few elements to which new elements are added at each step of the mapping protocol.

Examples

```
# --- get a matrix with raw-data
mydata <- matrix(rnorm(10000, mean = 0, sd = 3), ncol = 2)
mylabels <- apply(mydata, 1, function(row) round(sqrt(sum(row**2)), 0))
# --- create a \var{bdm} instance with our raw-data matrix
mybdm <- bdm.init('mydataset', mydata, labels = mylabels)
str(mybdm)
```

bdm.labels	<i>Get data-point clustering labels.</i>
------------	--

Description

Given that clusters are computed at grid-cell level, this function returns the clustering label for each data-point.

Usage

```
bdm.labels(bdm, layer = 1, merged = T)
```

Arguments

bdm	A <i>bdm</i> instance as generated by <code>bdm.init()</code> .
layer	The number of the t-SNE layer (1 by default).
merged	A logical value. If TRUE (default value) and the <i>bdm</i> has been merged, the data-point labelling indicate the number of the merged clusters. If <i>merged</i> is set to FALSE or the <i>bdm</i> has not been merged the data-point labels correspond to the top-level clustering.

Value

A vector of data-point clustering labels.

Examples

```
bdm.example()  
exMap.labels <- bdm.labels(exMap)
```

bdm.local	<i>Set/get default local machine name or IP address</i>
-----------	---

Description

Set/get default local machine name or IP address

Usage

```
bdm.local(dest = NULL)
```

Arguments

dest	Name or IP address of the local machine.
------	--

Value

The current value of *local*

Examples

```
# --- set default value of \var{local}
bdm.local('xxx.255.0.0')
bdm.local('mymachine.mydomain.cat')
```

bdm.mybdm

Set/get default path for mybdm

Description

Set/get default path for *mybdm*

Usage

```
bdm.mybdm(path = NULL)
```

Arguments

path Path to *mybdm*.

Value

The current path value to *mybdm*

Examples

```
# --- set default path for \var{mybdm}
bdm.mybdm('~mybdm')
```

bdm.pakde

*Perplexity-adaptive kernel density estimation***Description**

Starts the paKDE algorithm (second step of the mapping protocol).

Usage

```
bdm.pakde(bdm, layer = 1, threads = 2, type = "SOCK", ppx = 100,
          itr = 100, tol = 1e-05, g = 200, g.exp = 3)
```

Arguments

bdm	A <i>bdm</i> instance as generated by <code>bdm.init()</code> .
layer	The number of the t-SNE layer (1 by default).
threads	The number of parallel threads (in principle only limited by hardware resources, i.e. number of cores and available memory)
type	The type of cluster: 'SOCK' (default) for intra-node parallelization, 'MPI' (message passing interface) for inter-node parallelization.
ppx	The value of perplexity to compute similarities in the low-dimensional embedding (100 by default).
itr	The number of iterations for computing input similarities (100 by default).
tol	The tolerance lower bound for computing input similarities (1e-05 by default).
g	The resolution of the density space grid ($g * g$ cells, 200 by default).
g.exp	A numeric factor to avoid border effects. The grid limits will be expanded so as to enclose the density of the kernel of the most extreme embedded datapoints up to $g.exp$ times σ . By default, ($g.exp = 3$) the grid limits are expanded so as to enclose the 0.9986 of the probability mass of the most extreme kernels.

Details

When computing the *paKDE* the embedding area is discretized as a grid of size $g * g$ cells. In order to avoid border effects, the limits of the grid are expanded by default so as to enclose at least the 0.9986 of the cumulative distribution function (3σ) of the kernels of the most extreme mapped points in each direction.

The presence of outliers in the embedding can lead to undesired expansion of the grid limits. We can overcome this using lower values of *g.exp*. By setting $g.exp = 0$ the grid limits will be equal to the range of the embedding.

The values $g.exp = c(1, 2, 3, 4, 5, 6)$ enclose cdf values of 0.8413, 0.9772, 0.9986, 0.99996, 0.99999, 1.0 respectively.

Value

A copy of the input *bdm* instance with new element *bdm\$pakde* (paKDE output). *bdm\$pakde[[layer]]\$layer* = 'NC' stands for not computed layers.

Examples

```
# --- load mapped dataset
bdm.example()
# --- run paKDE
## Not run:
exMap <- bdm.pakde(exMap, threads = 4, ppx = 200, g = 200, g.exp = 3)

## End(Not run)
# --- plot paKDE output
bdm.plot(exMap)
```

bdm.plot

Mapping plots (ptSNE, paKDE, WTT)

Description

Mapping plots (ptSNE, paKDE, WTT)

Usage

```
bdm.plot(bdm, ptsne = FALSE, ptsne.cex = 0.5, ptsne.bg = "#FFFFFF",
  ptsne.pltt = NULL, pakde.pltt = NULL, pakde.lvls = 16,
  wtt.lwd = 1, plot.peaks = T, labels.cex = 1, layer = 1)
```

Arguments

<i>bdm</i>	A <i>bdm</i> instance as generated by <i>bdm.init()</i> or a list of them to make a comparative plot.
<i>ptsne</i>	A logical value. By default (<i>ptsne</i> = FALSE) the function depicts the plot of the last downstream step of the protocol that has been computed. With <i>ptsne</i> = TRUE the function plots back the ptSNE output.
<i>ptsne.cex</i>	The size of the mapped data-points in the ptSNE plot. Default value is <i>ptsne.cex</i> = 0.5.
<i>ptsne.bg</i>	The background colour of the ptSNE plot. Default value is <i>ptsne.bg</i> = #FFFFFF (white).
<i>ptsne.pltt</i>	A colour palette to show the clusters in the ptSNE plot by colouring the mapped data-points. By default (<i>ptsne.pltt</i> = NULL) the default palette is used.
<i>pakde.pltt</i>	A colour palette to show levels in the paKDE plot. By default (<i>pakde.pltt</i> = NULL) the default palette is used.
<i>pakde.lvls</i>	The number of levels of the density heat-map (16 by default).

<code>wtt.lwd</code>	The width of the watertrack lines (as set in <code>par()</code>).
<code>plot.peaks</code>	Logical value (TRUE by default). If set to TRUE and the up-stream step <code>bdm\$wtt()</code> is computed marks the peak of each cluster.
<code>labels.cex</code>	If <code>plot.peaks</code> is TRUE, the size of the labels of the clusters (as set in <code>par()</code>). By default <code>labels.cex=0.0</code> and the labels of the clusters are not depicted.
<code>layer</code>	The number of a layer (1 by default).

Value

None.

Examples

```
bdm.example()
exMap <- bdm.plot(exMap)
```

<code>bdm.ptsne</code>	<i>Parallelized t-SNE</i>
------------------------	---------------------------

Description

Starts the ptSNE algorithm (first step of the mapping protocol).

Usage

```
bdm.ptsne(bdm, threads = 3, type = "SOCK", layers = 2, rounds = 1,
  boost = 2, whiten = 4, input.dim = NULL, ppx = 100, itr = 100,
  tol = 1e-05, alpha = 0.5, Y.init = NULL, info = 1)
```

Arguments

<code>bdm</code>	A <i>bdm</i> instance as generated by <code>bdm.init()</code> .
<code>threads</code>	The number of parallel threads (in principle only limited by hardware resources, i.e. number of cores and available memory)
<code>type</code>	The type of cluster: 'SOCK' (default) for intra-node parallelization, 'MPI' (message passing interface) for inter-node parallelization.
<code>layers</code>	The number of layers (minimum 2, maximum the number of threads).
<code>rounds</code>	The number of rounds (2 by default).
<code>boost</code>	A running time accelerator factor. By default (<code>boost == 1</code>). See details.
<code>whiten</code>	Preprocessing of raw data. If <code>whiten = 4</code> (default value) raw data is preprocessed by computing the principal components (PCA) and whitening the rotated data. If <code>whiten = 3</code> only PCA is performed with NO whitening. If <code>whiten = 2</code> raw data is only centered and scaled. If <code>whiten = 1</code> raw data is only centered. If <code>whiten = 0</code> no preprocessing is performed at all.

<code>input.dim</code>	If <code>whiten</code> is TRUE, <code>input.dim</code> sets the number of principal components to be used as input dimensions. By default <code>input.dim = min(ncol(bdm\$data), 30)</code> . If <code>whiten</code> is FALSE all data columns will be used as input dimensions (<code>input.dim = ncol(bdm\$data)</code>).
<code>ppx</code>	The value of perplexity to compute similarities (100 by default).
<code>itr</code>	The number of iterations for computing input similarities (100 by default).
<code>tol</code>	The tolerance lower bound for computing input similarities (1e-05 by default).
<code>alpha</code>	The momentum factor (0.5 by default).
<code>Y.init</code>	A $n \times 2$ matrix with initial mapping positions. By default (NULL) will use random initial positions)
<code>info</code>	Progress output information: 1 yields inter-round results for progressive analytics, 0 disables intermediate results. Default value is 1.

Details

By default the algorithm is structured in \sqrt{n} epochs of \sqrt{z} iterations each, where n is the dataset size and z is the thread-size ($z = n * layers / threads$). The running time of the algorithm is then determined by $epochs * iters * t_i + epochs * t_e$ where t_i is the running time of a single iteration and t_e is the inter-epoch running time.

The *boost* factor is meant to reduce the running time. With $boost > 1$ the algorithm is structured in $n/boost$ epochs with $z * boost$ iterations each. This structure performs the same total number of iterations but arranged into a lower number of epochs, thus decreasing the total running time to $epochs * iters * t_i + 1/boost * epochs * t_e$. When the number of threads is high, the inter-epoch time can be high, in particular when using 'MPI' parallelization, thus, reducing the number of epochs can result in a significant reduction of the total running time. The counterpart is that increasing the number of iterations per epoch might result in a lack of convergence, thus the *boost* factor must be used with caution. To the most of our knowledge using values up to $boost = 2.5$ is generally safe.

Value

A copy of the input *bdm* instance with new element *bdm\$ptsne* (t-SNE output).

Examples

```
# --- load example dataset
bdm.example()
# --- perform ptSNE
## Not run:
exMap <- bdm.ptsne(exMap, threads = 10, layers = 2, rounds = 2, ppx = 200)

## End(Not run)
# --- plot the Cost function
bdm.cost(exMap)
# --- plot ptSNE output
bdm.plot(exMap)
```

bdm.qMap	<i>ptSNE quantile-maps</i>
----------	----------------------------

Description

Shows the mapping of quantitative variables into the embedding space.

Usage

```
bdm.qMap(bdm, layer = 1, data = NULL, labels = NULL, subset = NULL,
         levels = 16, cex = 0.3)
```

Arguments

bdm	A <i>bdm</i> instance as generated by <code>bdm.init()</code> .
layer	The number of a layer (1 by default).
data	A matrix/data.frame to be mapped. By default, the input data <code>bdm\$data</code> is mapped.
labels	If available, labels can be included as a separate vector of length equal to <code>nrow(dSet.data)</code> . Label values are factorized as <code>as.numeric(as.factor(labels))</code> .
subset	A numeric vector with the indexes of a subset of data. Data-points in the subset are heat-mapped and the rest are shown in light grey. By default all data-points are heat-mapped.
levels	The number of levels of the heat-map (16 by default).
cex	The size of the data-points (as in <code>par()</code>).

Value

None.

Examples

```
bdm.example()
bdm.qMap(exMap)
# --- show only components (1, 2, 4, 8) of the GMM
bdm.qMap(exMap, subset = which(exMap$lbls %in% c(1, 4, 8, 16)))
```

bdm.save	<i>Save bdm instance</i>
----------	--------------------------

Description

Saves a *bdm* instance with default path/file names, as given by `bdm.mybdm()/bdm.fName(bdm)`. Default file name is generated based on `bdm$dSet` and `ptSNE` main parameters (threads, layers, boost, rounds, perplexity). The purpose of functions `bdm.save()` and `bdm.scp()` used with `bdm.fName()` is to ease the task of working/organizing multiple runs on the same dataset.

Usage

```
bdm.save(...)
```

Arguments

... A *bdm* instance as generated by `bdm.init()`.

Value

None

Examples

```
# --- get a matrix with raw-data
mydata <- cbind(rnorm(10000, mean = 0, sd = 3), ncol = 2)
mylabels <- apply(mydata, 1, function(row) round(sqrt(sum(row**2)), 0))
# --- create a \var{bdm} instance with our raw-data matrix
mybdm <- bdm.init('mydataset', mydata, labels = mylabels)
str(mybdm)
# --- save it
## Not run:
bdm.save(mybdm)

## End(Not run)
```

bdm.scp	<i>Transfer bdm instance to a remote machine.</i>
---------	---

Description

Transfers a *bdm* instance to a remote machine. By default a file name is generated based on `bdm$dSet` and `t-SNE` main parameters (threads, layers, rounds, perplexity). The purpose of functions `bdm.save()` and `bdm.scp()` used with `bdm.fName()` is to ease the task of working/organizing multiple runs on the same dataset.

Usage

```
bdm.scp(..., dest = NULL)
```

Arguments

```
...           A bdm instance as generated by bdm.init().
dest         The name or IP address of a remote machine where to transfer the file of the
             bdm instance. By default is send to bdm.local() environment variable.
```

Value

```
None
```

Examples

```
## Not run:
# --- load example
bdm.example()
# --- scp to \var{bdm.local()} with default file name
bdm.scp(exMap)
# --- scp to IP address 'xxx.xxx.0.0' with default file name
bdm.scp(exMap, dest = 'xxx.xxx.0.0')

## End(Not run)
```

```
bdm.wtt
```

```
Watertrack transform (WTT)
```

Description

Starts the WTT algorithm (third setp of the mapping protocol).

Usage

```
bdm.wtt(bdm, layer = 1)
```

Arguments

```
bdm          A bdm instance as generated by bdm.init().
layer       The number of the t-SNE layer (1 by default).
```

Details

This function requires the up-stream step *bdm.pakde()*.

Value

A copy of the input *bdm* instance with *bdm\$wtt* (WTT output). *bdm\$wtt[[layer]]\$layer = 'NC'* stands for not computed layers.

Examples

```
# --- load mapped dataset
bdm.example()
# --- perform WTT
exMap <- bdm.wtt(exMap)
# --- plot WTT output
bdm.plot(exMap)
```

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