

Package ‘EmbedSOM’

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Title Fast Embedding Guided by Self-Organizing Map

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Imports ggplot2, igraph, Matrix, Rtsne, umap, uwot

Description Provides a smooth mapping of multidimensional points into low-dimensional space defined by a self-organizing map. Designed to work with 'FlowSOM' and flow-cytometry use-cases. See Kratochvil et al. (2019) <[doi:10.12688/f1000research.21642.1](https://doi.org/10.12688/f1000research.21642.1)>.

License GPL (>= 3)

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Contents

ClusterPalette	2
EmbedSOM	3
ExprColors	4
ExpressionGradient	5

ExpressionPalette	6
GQTSOM	6
GraphCoords	7
Initialize_PCA	8
kMeansMap	8
kNNCoords	9
MapDataToCodes	10
MSTCoords	10
NormalizeColor	11
PlotData	12
PlotDefault	13
PlotEmbed	13
PlotGG	15
PlotId	15
RandomMap	16
SOM	16
tSNECoords	18
UMAPCoords	19
UMatrixCoords	19
uwotCoords	20

Index	21
--------------	-----------

ClusterPalette	<i>An acceptable cluster color palette</i>
----------------	--

Description

An acceptable cluster color palette

Usage

```
ClusterPalette(n, vcycle = c(1, 0.7), scycle = c(0.7, 1), alpha = 1)
```

Arguments

n	How many colors to generate
vcycle, scycle	Small vectors with cycles of saturation/value for hsv
alpha	Opacity of the colors

Examples

```
EmbedSOM::ClusterPalette(10)
```

EmbedSOM

Process the cells with SOM into a nice embedding

Description

Process the cells with SOM into a nice embedding

Usage

```
EmbedSOM(
  data = NULL,
  map = NULL,
  fsom = NULL,
  smooth = NULL,
  k = NULL,
  adjust = NULL,
  importance = NULL,
  coordsFn = NULL,
  coords = NULL,
  emcoords = NULL,
  emcoords.pow = 1,
  parallel = F,
  threads = if (parallel) 0 else 1
)
```

Arguments

<code>data</code>	Data matrix with points that optionally overrides the one from <code>fsom\$data</code>
<code>map</code>	Map object in FlowSOM format, to optionally override <code>fsom\$map</code>
<code>fsom</code>	FlowSOM object with a built SOM (used if <code>data</code> or <code>map</code> are missing)
<code>smooth</code>	Produce smoother (positive values) or more rough approximation (negative values).
<code>k</code>	How many neighboring landmarks (e.g. SOM nodes) to take into the whole computation
<code>adjust</code>	How much non-local information to remove from the approximation
<code>importance</code>	Scaling of the landmarks, will be used to scale the incoming data (should be same as used for training the SOM or to select the landmarks)
<code>coordsFn</code>	A coordinates-generating function (e.g. <code>tSNECoords()</code>) that overrides the existing <code>map\$grid</code> .
<code>coords</code>	A matrix of embedding-space coordinates that correspond to <code>map\$codes</code> (i.e. the "embedded landmarks"). Overrides <code>map\$grid</code> if not NULL.
<code>emcoords</code>	Provided for backwards compatibility, will be removed. Use <code>coords</code> and <code>coordsFn</code> instead.

emcoords.pow	Provided for backwards compatibility, will be removed. Use a parametrized coordsFn instead.
parallel	Boolean flag whether the computation should be parallelized (this flag is just a nice name for threads and does not do anything directly – default FALSE sets threads=1, TRUE sets threads=0)
threads	Number of threads used for computation, 0 chooses hardware concurrency, 1 (default) turns off parallelization.

Value

matrix with 2D or 3D coordinates of the embedded data, depending on the map

Examples

```
d <- cbind(rnorm(10000), 3*runif(10000), rexp(10000))
colnames(d) <- paste0("col",1:3)
map <- EmbedSOM::SOM(d, xdim=10, ydim=10)
e <- EmbedSOM::EmbedSOM(data=d, map=map)
EmbedSOM::PlotEmbed(e, data=d, 'col1', pch=16)
```

ExprColors	<i>Generate colors for multi-color marker expression labeling in a single plot</i>
------------	--

Description

Generate colors for multi-color marker expression labeling in a single plot

Usage

```
ExprColors(
  exprs,
  base = exp(1),
  scale = 1,
  cutoff = 0,
  pow = NULL,
  col = ClusterPalette(dim(exprs)[2], alpha = alpha),
  nocolor = grDevices::rgb(0.75, 0.75, 0.75, alpha/2),
  alpha = 0.5
)
```

Arguments

exprs	Matrix-like object with marker expressions (extract it manually from your data)
base, scale	Base(s) and scale(s) for softmax (convertible to numeric vectors of size 1+ncol(exprs))
cutoff	Gray level (expressed in sigmas of the sample distribution)

pow	Obsolete, now renamed to scale.
col	Colors to use, defaults to colors taken from 'ClusterPalette'
nocolor	The color to use for sub-gray-level expression, default gray.
alpha	Default alpha value.

Examples

```
d <- cbind(rnorm(1e5), rexp(1e5))
EmbedSOM::PlotEmbed(d, col=EmbedSOM::ExprColors(d, pow=2))
```

ExpressionGradient *The ggplot2 scale gradient from ExpressionPalette.*

Description

The ggplot2 scale gradient from ExpressionPalette.

Usage

```
ExpressionGradient(...)
```

Arguments

... Arguments passed to [ggplot2::scale_color_gradientn\(\)](#)

Examples

```
library(EmbedSOM)
library(ggplot2)

# simulate a simple dataset
e <- cbind(rnorm(10000), rnorm(10000))

data <- data.frame(Val=log(1+e[,1]^2+e[,2]^2))
PlotGG(e, data=data) +
  geom_point(aes_string(color="Val"), alpha=.5) +
  ExpressionGradient(guide=FALSE)
```

ExpressionPalette	<i>Marker expression palette generator based off ColorBrewer's RdYlBu, only better for plotting of half-transparent cells</i>
-------------------	---

Description

Marker expression palette generator based off ColorBrewer's RdYlBu, only better for plotting of half-transparent cells

Usage

```
ExpressionPalette(n, alpha = 1)
```

Arguments

n	How many colors to generate
alpha	Opacity of the colors

Examples

```
EmbedSOM::ExpressionPalette(10)
```

GQTSOM	<i>Train a Growing Quadtree Self-Organizing Map</i>
--------	---

Description

Train a Growing Quadtree Self-Organizing Map

Usage

```
GQTSOM(
  data,
  init.dim = c(3, 3),
  target_codes = 100,
  rlen = 10,
  radius = c(sqrt(sum(init.dim^2)), 0.5),
  epochRadii = seq(radius[1], radius[2], length.out = rlen),
  coords = NULL,
  codes = NULL,
  coordsFn = NULL,
  importance = NULL,
  distf = 2,
  nhbr.distf = 2,
  noMapping = F,
  parallel = F,
  threads = if (parallel) 0 else 1
)
```

Arguments

<code>data</code>	Input data matrix
<code>init.dim</code>	Initial size of the SOM, default <code>c(3, 3)</code>
<code>target_codes</code>	Make the SOM grow linearly to at most this amount of nodes (default 100)
<code>r.len</code>	Number of training iterations
<code>radius</code>	Start and end training radius, as in <code>SOM()</code>
<code>epochRadii</code>	Precise radii for each epoch (must be of length <code>r.len</code>)
<code>coords</code>	Quadtree coordinates of the initial SOM nodes.
<code>codes</code>	Initial codebook
<code>coordsFn</code>	Function to generate/transform grid coordinates (e.g. <code>tSNECoords()</code>). If NULL (default), the grid is the 2D coordinates of GQTSOM map.
<code>importance</code>	Weights of input data dimensions
<code>distf</code>	Distance measure to use in input data space (1=manhattan, 2=euclidean, 3=chebyshev, 4=cosine)
<code>nhbr.distf</code>	Distance measure to use in output space (as in <code>distf</code>)
<code>noMapping</code>	If TRUE, do not compute the assignment of input data to SOM nodes
<code>parallel</code>	Parallelize the training by setting appropriate threads. Defaults to FALSE.
<code>threads</code>	Number of threads to use for training. Defaults to 0 (chooses maximum available hardware threads) if <code>parallel=TRUE</code> or 1 (single thread) if <code>parallel=FALSE</code> .

GraphCoords

Add Kamada-Kawai-generated embedding coordinates to the map

Description

This uses a complete graph on the map codebook, which brings overcrowding problems. It is therefore useful to transform the distances for avoiding that (e.g. by exponentiating them slightly using `distFn` function).

Usage

```
GraphCoords(
  dim = NULL,
  dist.method = NULL,
  distFn = function(x) x,
  layoutFn = igraph::layout_with_kk
)
```

Arguments

<code>dim</code>	Dimension of the result (passed to <code>layoutFn</code>)
<code>dist.method</code>	The method to compute distances, passed to <code>stats::dist()</code> as parameter <code>method</code>
<code>distFn</code>	Custom transformation function of the distance matrix
<code>layoutFn</code>	<code>igraph</code> -compatible graph layouting function (default <code>igraph::layout_with_kk</code>)

Value

a function that transforms the map, usable as coordsFn parameter

Initialize_PCA	<i>Create a grid from first 2 PCA components</i>
----------------	--

Description

Create a grid from first 2 PCA components

Usage

```
Initialize_PCA(data, xdim, ydim, zdim = NULL)
```

Arguments

data matrix in which each row represents a point
 xdim, ydim, zdim Dimensions of the SOM grid

Value

array containing the selected selected rows

kMeansMap	<i>Create a map from k-Means clusters</i>
-----------	---

Description

May give better results than 'RandomMap' on data where random sampling is complicated. This does not use actual kMeans clustering, but re-uses the batch version of [SOM\(\)](#) with tiny radius (which makes it work the same as kMeans). In consequence, the speedup of SOM function is applied here as well. Additionally, because we don't need that amount of clustering precision, parameters 'batch=F, rlen=1' may give a satisfactory result very quickly.

Usage

```
kMeansMap(data, k, coordsFn, batch = T, ...)
```

Arguments

data Input data matrix, with individual data points in rows
 k How many points to sample
 coordsFn a function to generate embedding coordinates (default none)
 batch Use batch-SOM training (effectively kMeans, default TRUE)
 ... Passed to [SOM\(\)](#), useful e.g. for 'parallel=T' or 'rlen=5'

Value

map object (without the grid, if coordsFn was not specified)

Examples

```
d <- iris[,1:4]
EmbedSOM::PlotEmbed(
  EmbedSOM::EmbedSOM(
    data = d,
    map = EmbedSOM::kMeansMap(d, 10, EmbedSOM::GraphCoords()),
    pch=19, clust=iris[,5]
  )
)
```

kNNCoords

Add KNN-topology-based embedding coordinates to the map

Description

Internally, this does not use `FNN::get.knn()` anymore.

Usage

```
kNNCoords(
  k = 4,
  dim = NULL,
  dist.method = NULL,
  distFn = function(x) x,
  layoutFn = igraph::layout_with_kk
)
```

Arguments

k	Size of the neighborhoods (default 4)
dim	Dimension of the result (passed to layoutFn)
dist.method	The method to compute distances, passed to <code>stats::dist()</code> as parameter method
distFn	Custom transformation function of the distance matrix
layoutFn	iGraph-compatible graph layouting function (default <code>igraph::layout_with_kk</code>)

Value

a function that transforms the map, usable as coordsFn parameter

MapDataToCodes	<i>Assign nearest node to each datapoint</i>
----------------	--

Description

Assign nearest node to each datapoint

Usage

```
MapDataToCodes(
  codes,
  data,
  distf = 2,
  parallel = F,
  threads = if (parallel) 0 else 1
)
```

Arguments

codes	matrix with nodes of the SOM
data	datapoints to assign
distf	Distance function (1=manhattan, 2=euclidean, 3=chebyshev, 4=cosine)
threads, parallel	Use parallel computation (see SOM())

Value

array with nearest node id for each datapoint

MSTCoords	<i>Add MST-style embedding coordinates to the map</i>
-----------	---

Description

Add MST-style embedding coordinates to the map

Usage

```
MSTCoords(
  dim = NULL,
  dist.method = NULL,
  distFn = function(x) x,
  layoutFn = igraph::layout_with_kk
)
```

Arguments

dim	Dimension of the result (passed to layoutFn)
dist.method	The method to compute distances, passed to <code>stats::dist()</code> as parameter method
distFn	Custom transformation function of the distance matrix
layoutFn	iGraph-compatible graph layouting function (default <code>igraph::layout_with_kk()</code>)

Value

a function that transforms the map, usable as coordsFn parameter

NormalizeColor	<i>Helper for computing colors for embedding plots</i>
----------------	--

Description

Helper for computing colors for embedding plots

Usage

```
NormalizeColor(data, low = NULL, high = NULL, pow = 0, sds = 1)
```

Arguments

data	Vector of scalar values to normalize between 0 and 1
low, high	Originally quantiles for clamping the color. Only kept for backwards compatibility, now ignored.
pow	The scaled data are transformed to $\text{data}^{(2^{\text{pow}})}$. If set to 0, nothing happens. Positive values highlight differences in the data closer to 1, negative values highlight differences closer to 0.
sds	Inverse scale factor for measured standard deviation (greater value makes data look more extreme)

Examples

```
EmbedSOM::NormalizeColor(c(1,100,500))
```

PlotData

Export a data frame for plotting with marker intensities and density.

Description

Export a data frame for plotting with marker intensities and density.

Usage

```
PlotData(  
  embed,  
  fsom,  
  data = fsom$data,  
  cols,  
  names,  
  normalize = cols,  
  pow = 0,  
  sds = 1,  
  vf = PlotId,  
  density = "Density",  
  densBins = 256,  
  densLimit = NULL,  
  fdens = sqrt  
)
```

Arguments

embed, fsom, data, cols	The embedding data, columns to select
names	Column names for output
normalize	List of columns to normalize using NormalizeColor() , default all
pow, sds	Parameters for the normalization
vf	Custom value-transforming function
density	Name of the density column
densBins	Number of bins for density calculation
densLimit	Upper limit of density (prevents outliers)
fdens	Density-transforming function; default sqrt

PlotDefault	<i>Default plot</i>
-------------	---------------------

Description

Default plot

Usage

```
PlotDefault(pch = ".", cex = 1, ...)
```

Arguments

pch, cex, ... correctly defaulted and passed to 'plot'

PlotEmbed	<i>Helper function for plotting the embedding</i>
-----------	---

Description

Convenience plotting function. Takes the embed matrix which is the output of [EmbedSOM\(\)](#), together with a multitude of arguments that set how the plotting is done.

Usage

```
PlotEmbed(  
  embed,  
  value = 0,  
  red = 0,  
  green = 0,  
  blue = 0,  
  fr = PlotId,  
  fg = PlotId,  
  fb = PlotId,  
  fv = PlotId,  
  powr = 0,  
  powg = 0,  
  powb = 0,  
  powv = 0,  
  sdsr = 1,  
  sdsg = 1,  
  sdsb = 1,  
  sdsv = 1,  
  clust = NULL,  
  nbin = 256,
```

```

maxDens = NULL,
fdens = sqrt,
limit = NULL,
alpha = NULL,
fsom,
data,
col,
cluster.colors = ClusterPalette,
expression.colors = ExpressionPalette,
na.color = grDevices::rgb(0.75, 0.75, 0.75, if (is.null(alpha)) 0.5 else alpha/2),
plotf = PlotDefault,
...
)

```

Arguments

embed	The embedding from EmbedSOM() , or generally any 2-column matrix of coordinates
value	The column of data to use for coloring the plotted points
red, green, blue	The same, for individual RGB components
fv, fr, fg, fb	Functions to transform the values before they are normalized
powv, powr, powg, powb	Passed to corresponding NormalizeColor() calls as pow
sdsv, sdsr, sdsg, sdsb	Passed to NormalizeColor() as sds
clust	Cluster labels (used as a factor)
nbin, maxDens, fdens	Parameters of density calculation, see PlotData()
limit	Low/high offset for NormalizeColor() (obsolete&ignored, will be removed)
alpha	Default alpha value of points
fsom	FlowSOM object
data	Data matrix, taken from fsom parameter by default
col	Overrides the computed point colors with exact supplied colors.
cluster.colors	Function to generate cluster colors, default ClusterPalette()
expression.colors	Function to generate expression color scale, default ExpressionPalette()
na.color	Color to assign to NA values
plotf	Plot function, defaults to graphics::plot() slightly decorated with pch='.', cex=1
...	Extra params passed to the plot function

Examples

```
EmbedSOM::PlotEmbed(cbind(rnorm(1e5), rnorm(1e5)))
```

PlotGG	<i>Wrap PlotData result in ggplot object.</i>
--------	---

Description

This creates a ggplot2 object for plotting.

Usage

```
PlotGG(embed, ...)
```

Arguments

embed	Embedding data
...	Extra arguments passed to PlotData()

Examples

```
library(EmbedSOM)
library(ggplot2)

# simulate a simple dataset
e <- cbind(rnorm(10000), rnorm(10000))

PlotGG(e, data=data.frame(Expr=runif(10000))) +
  geom_point(aes_string(color="Expr"))
```

PlotId	<i>Identity on whatever</i>
--------	-----------------------------

Description

Identity on whatever

Usage

```
PlotId(x)
```

Arguments

x	Just the x.
---	-------------

Value

The x.

RandomMap	<i>Create a map by randomly selecting points</i>
-----------	--

Description

Create a map by randomly selecting points

Usage

```
RandomMap(data, k, coordsFn)
```

Arguments

data	Input data matrix, with individual data points in rows
k	How many points to sample
coordsFn	a function to generate embedding coordinates (default none)

Value

map object (without the grid, if coordsFn was not specified)

Examples

```
d <- iris[,1:4]
EmbedSOM::PlotEmbed(
  EmbedSOM::EmbedSOM(
    data = d,
    map = EmbedSOM::RandomMap(d, 30, EmbedSOM::GraphCoords()),
    pch=19, clust=iris[,5]
  )
)
```

SOM	<i>Build a self-organizing map</i>
-----	------------------------------------

Description

Build a self-organizing map

Usage

```

SOM(
  data,
  xdim = 10,
  ydim = 10,
  zdim = NULL,
  batch = F,
  rlen = 10,
  alphaA = c(0.05, 0.01),
  radiusA = stats::quantile(nhbrdist, 0.67) * c(1, 0),
  alphaB = alphaA * c(-negAlpha, -0.1 * negAlpha),
  radiusB = negRadius * radiusA,
  negRadius = 1.33,
  negAlpha = 0.1,
  epochRadii = seq(radiusA[1], radiusA[2], length.out = rlen),
  init = FALSE,
  initf = Initialize_PCA,
  distf = 2,
  codes = NULL,
  importance = NULL,
  coordsFn = NULL,
  nhbr.method = "maximum",
  noMapping = F,
  parallel = F,
  threads = if (parallel) 0 else 1
)

```

Arguments

<code>data</code>	Matrix containing the training data
<code>xdim</code>	Width of the grid
<code>ydim</code>	Hight of the grid
<code>zdim</code>	Depth of the grid, causes the grid to be 3D if set
<code>batch</code>	Use batch training (default FALSE chooses online training, which is more like FlowSOM)
<code>rlen</code>	Number of training epochs; or number of times to loop over the training data in online training
<code>alphaA</code>	Start and end learning rate for online learning (only for online training)
<code>radiusA</code>	Start and end radius
<code>alphaB</code>	Start and end learning rate for the second radius (only for online training)
<code>radiusB</code>	Start and end radius (only for online training; make sure it is larger than radiusA)
<code>negRadius</code>	easy way to set radiusB as a multiple of default radius (use lower value for higher dimensions)
<code>negAlpha</code>	the same for alphaB
<code>epochRadii</code>	Vector of length <code>rlen</code> with precise epoch radii (only for batch training)

<code>init</code>	Initialize cluster centers in a non-random way
<code>initf</code>	Use the given initialization function if <code>init==T</code> (default: <code>Initialize_PCA</code>)
<code>distf</code>	Distance function (1=manhattan, 2=euclidean, 3=chebyshev, 4=cosine)
<code>codes</code>	Cluster centers to start with
<code>importance</code>	array with numeric values. Columns of data will be scaled according to importance.
<code>coordsFn</code>	Function to generate/transform grid coordinates (e.g. <code>tSNECoords()</code>). If NULL (default), the grid is the canonical SOM grid.
<code>nhbr.method</code>	Way of computing grid distances, passed as <code>method=</code> to <code>stats::dist()</code> function. Defaults to maximum (square neighborhoods); use euclidean for round neighborhoods.
<code>noMapping</code>	If TRUE, do not compute the mapping (default FALSE). Makes the process quicker by 1 rlen.
<code>parallel</code>	Parallelize the batch training by setting appropriate threads. Defaults to FALSE. Always use <code>batch=TRUE</code> for fully parallelized version, online training is not parallelizable. Passed to <code>MapDataToCodes()</code> .
<code>threads</code>	Number of threads of the batch training (has no effect on online training). Defaults to 0 (chooses maximum available hardware threads) if <code>parallel==TRUE</code> or 1 (single thread) if <code>parallel==FALSE</code> . Passed to <code>MapDataToCodes()</code> .

Value

A map useful for embedding (`EmbedSOM()` function) or further analysis, e.g. clustering.

See Also

`FlowSOM::SOM`

tSNECoords

Add tSNE-based coordinates to a map

Description

Add tSNE-based coordinates to a map

Usage

```
tSNECoords(dim = NULL, tSNEFn = Rtsne::Rtsne, ...)
```

Arguments

<code>dim</code>	Dimension of the result (passed to <code>tSNEFn</code> as <code>dims</code>)
<code>tSNEFn</code>	tSNE function to run (default <code>Rtsne::Rtsne</code>)
<code>...</code>	passed to <code>tSNEFn</code>

Value

a function that transforms the map, usable as coordsFn parameter

UMAPCoords	<i>Add UMAP-based coordinates to a map</i>
------------	--

Description

Add UMAP-based coordinates to a map

Usage

```
UMAPCoords(dim = NULL, UMAPFn = NULL)
```

Arguments

dim	Dimension of the result (passed to UMAPFn as n_components)
UMAPFn	UMAP function to run (default umap::umap configured by umap::umap.defaults)

Value

a function that transforms the map, usable as coordsFn parameter

UMatrixCoords	<i>Add U-Matrix-optimized embedding coordinates to the map</i>
---------------	--

Description

The map must already contain a SOM grid with corresponding xdim,ydim (possibly zdim)

Usage

```
UMatrixCoords(
  dim = NULL,
  dist.method = NULL,
  distFn = function(x) x,
  layoutFn = igraph::layout_with_kk
)
```

Arguments

dim	Dimension of the result (passed to layoutFn)
dist.method	The method to compute distances, passed to stats::dist() as parameter method
distFn	Custom transformation function of the distance matrix
layoutFn	iGraph-compatible graph layouting function (default igraph::layout_with_kk)

Value

a function that transforms the map, usable as 'coordsFn' parameter

uwotCoords

Add UMAP-based coordinates to a map, using the 'uwot' package

Description

Add UMAP-based coordinates to a map, using the 'uwot' package

Usage

```
uwotCoords(dim = NULL, uwotFn = uwot::umap, ...)
```

Arguments

dim	Dimension of the result (passed to uwotFn as dims)
uwotFn	UMAP function to run (default uwot::umap)
...	passed to uwotFn

Value

a function that transforms the map, usable as coordsFn parameter

Index

ClusterPalette, [2](#)
ClusterPalette(), [14](#)

EmbedSOM, [3](#)
EmbedSOM(), [13](#), [14](#), [18](#)
ExprColors, [4](#)
ExpressionGradient, [5](#)
ExpressionPalette, [6](#)
ExpressionPalette(), [14](#)

FNN::get.knn(), [9](#)

ggplot2::scale_color_gradientn(), [5](#)
GQTSOM, [6](#)
GraphCoords, [7](#)
graphics::plot(), [14](#)

igraph::layout_with_kk, [7](#), [9](#), [19](#)
igraph::layout_with_kk(), [11](#)
Initialize_PCA, [8](#)

kMeansMap, [8](#)
kNNCoords, [9](#)

MapDataToCodes, [10](#)
MapDataToCodes(), [18](#)
MSTCoords, [10](#)

NormalizeColor, [11](#)
NormalizeColor(), [12](#), [14](#)

PlotData, [12](#)
PlotData(), [14](#), [15](#)
PlotDefault, [13](#)
PlotEmbed, [13](#)
PlotGG, [15](#)
PlotId, [15](#)

RandomMap, [16](#)
Rtsne::Rtsne, [18](#)

SOM, [16](#)
SOM(), [7](#), [8](#), [10](#)
stats::dist(), [7](#), [9](#), [11](#), [18](#), [19](#)
tSNECoords, [18](#)
tSNECoords(), [3](#), [7](#), [18](#)
umap::umap, [19](#)
umap::umap.defaults, [19](#)
UMAPCoords, [19](#)
UMatrixCoords, [19](#)
uwot::umap, [20](#)
uwotCoords, [20](#)