

Package ‘GeneralizedUmatrix’

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Type Package

Title Credible Visualization for Two-Dimensional Projections of Data

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Description Projections are common dimensionality reduction methods, which represent high-dimensional data in a two-dimensional space. However, when restricting the output space to two dimensions, which results in a two dimensional scatter plot (projection) of the data, low dimensional similarities do not represent high dimensional distances coersively [Thrun, 2018] <[DOI:10.1007/978-3-658-20540-9](https://doi.org/10.1007/978-3-658-20540-9)>. This could lead to a misleading interpretation of the underlying structures [Thrun, 2018]. By means of the 3D topographic map the generalized Umatrix is able to depict errors of these two-dimensional scatter plots. The package is derived from the book of Thrun, M.C.: “Projection Based Clustering through Self-Organization and Swarm Intelligence” (2018) <[DOI:10.1007/978-3-658-20540-9](https://doi.org/10.1007/978-3-658-20540-9)> and the main algorithm called simplified self-organizing map for dimensionality reduction methods is published in <[DOI:10.1016/j.mex.2020.101093](https://doi.org/10.1016/j.mex.2020.101093)>.

License GPL-3

Imports Rcpp (>= 1.0.8), RcppParallel (>= 5.1.4), ggplot2

Suggests DataVisualizations, rgl, grid, mgcv, png, reshape2, fields, ABCanalysis, plotly, deldir, methods, knitr (>= 1.12), rmarkdown (>= 0.9)

LinkingTo Rcpp, RcppArmadillo, RcppParallel

Depends R (>= 3.0)

NeedsCompilation yes

SystemRequirements C++11, GNU make, pandoc (>=1.12.3, needed for vignettes)

LazyLoad yes

LazyData TRUE

URL <https://www.deepbionics.org>

Encoding UTF-8

VignetteBuilder knitr

BugReports <https://github.com/Mthrun/GeneralizedUmatrix/issues>

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 GeneralizedUmatrix-package

Credible Visualization for Two-Dimensional Projections of Data

Description

Projections are common dimensionality reduction methods, which represent high-dimensional data in a two-dimensional space. However, when restricting the output space to two dimensions, which results in a two dimensional scatter plot (projection) of the data, low dimensional similarities do not represent high dimensional distances coercively [Thrun, 2018] <DOI: 10.1007/978-3-658-20540-9>. This could lead to a misleading interpretation of the underlying structures [Thrun, 2018]. By means of the 3D topographic map the generalized Umatrix is able to depict errors of these two-dimensional scatter plots. The package is derived from the book of Thrun, M.C.: "Projection Based Clustering through Self-Organization and Swarm Intelligence" (2018) <DOI:10.1007/978-3-658-20540-9> and the main algorithm called simplified self-organizing map for dimensionality reduction methods is published in <DOI: 10.1016/j.mex.2020.101093>.

Details

For a brief introduction to **GeneralizedUmatrix** please see the vignette [Introduction of the Generalized Umatrix Package](#).

For further details regarding the generalized Umatrix see [Thrun, 2018], chapter 4-5, or [Thrun/Ultsch, 2020].

If you want to verify your clustering result externally, you can use Heatmap or SilhouettePlot of the CRAN package DataVisualizations.

Index of help topics:

CalcUstarmatrix	Calculate the U*matrix for a given Umatrix and Pmatrix.
Chainlink	Chainlink is part of the Fundamental Clustering Problem Suit (FCPS) [Thrun/Ultsch, 2020].
DefaultColorSequence	Default color sequence for plots
Delta3DWeightsC	intern function
EsomNeuronsAsList	Converts wts data (EsomNeurons) into the list form
ExtendToroidalUmatrix	Extend Toroidal Umatrix
GeneralizedUmatrix	Generalized U-Matrix for Projection Methods published in [Thrun/Ultsch, 2020]
GeneralizedUmatrix-package	Credible Visualization for Two-Dimensional Projections of Data
GeneratePmatrix	Generates the P-matrix
ListAsEsomNeurons	Converts List to WTS
LowLand	LowLand
NormalizeUmatrix	Normalize Umatrix
ReduceToLowLand	ReduceToLowLand

TopviewTopographicMap	Topview of Topographic Map ind 2D
Uheights4Data	Uheights4Data
UmatrixColormap	U-Matrix colors
UniqueBestMatchingUnits	UniqueBestMatchingUnits
XYcoords2LinesColumns	XYcoords2LinesColumns(X,Y) Converts points given as x(i),y(i) coordinates to integer coordinates Columns(i),Lines(i)
addRowWiseC	intern function
plotTopographicMap	Visualizes the Generalized U-matrix in 3D
sESOM4BMUs	simplified ESOM
setdiffMatrix	setdiffMatrix shortens Matrix2Curt by those rows that are in both matrices.
trainstepC	internal function for s-esom
upscaleUmatrix	Upscale a Umatrix grid

Author(s)

Michal Thrun

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References

[Thrun/Ultsch, 2020] Thrun, M. C., & Ultsch, A.: Uncovering High-Dimensional Structures of Projections from Dimensionality Reduction Methods, *MethodsX*, Vol. in press, pp. 101093. doi 10.1016/j.mex.2020.101093, 2020.

[Thrun, 2018] Thrun, M. C.: Projection Based Clustering through Self-Organization and Swarm Intelligence, doctoral dissertation 2017, Springer, Heidelberg, ISBN: 978-3-658-20539-3, doi:10.1007/9783658205409, 2018.

[Ultsch/Thrun, 2017] Ultsch, A., & Thrun, M. C.: Credible Visualizations for Planar Projections, in Cottrell, M. (Ed.), 12th International Workshop on Self-Organizing Maps and Learning Vector Quantization, Clustering and Data Visualization (WSOM), IEEE Xplore, France, 2017.

Examples

```
data("Chainlink")
Data=Chainlink$Data
Cls=Chainlink$Cls
InputDistances=as.matrix(dist(Data))
res=cmdscale(d=InputDistances, k = 2, eig = TRUE, add = FALSE, x.ret = FALSE)
ProjectedPoints=as.matrix(res$points)
#see also ProjectionBasedClustering package for other common projection methods
#see DatabionicsWorm for projection method without parameters or objective function
# ProjectedPoints=DatabionicsWorm::Pswarm(Data)$ProjectedPoints

resUmatrix=GeneralizedUmatrix(Data,ProjectedPoints)
plotTopographicMap(resUmatrix$Umatrix,resUmatrix$Bestmatches,Cls)

##Interactive Island Generation
```

```
## from a tiled Umatrix (toroidal assumption)
## Not run:
Imx = ProjectionBasedClustering::interactiveGeneralizedUmatrixIsland(resUmatrix$Umatrix,
resUmatrix$Bestmatches)
plotTopographicMap(resUmatrix$Umatrix,

resUmatrix$Bestmatches, Imx = Imx)

## End(Not run)
#External Verification
## Not run:

DataVisualizations::Heatmap(Data,Cls)
#if spherical cluster strcuture
DataVisualizations::SilhouettePlot(Data,Cls)

## End(Not run)
```

addRowWiseC

intern function

Description

Adds the Vector DataPoint to every row of the matrix WeightVectors

Usage

```
addRowWiseC(WeightVectors,DataPoint)
```

Arguments

WeightVectors WeightVectors. n weights with m components each

DataPoint Vector with m components

Value

WeightVectors [1:m,1:n]

CalcUstarmatrix	<i>Calculate the U*matrix for a given Umatrix and Pmatrix.</i>
-----------------	--

Description

Calculate the U*matrix for a given Umatrix and Pmatrix.

Arguments

Umatrix	[1:Lines,1:Column] Local averages of distances at each point of the trained-GridWts[1:Lines,1:Column,1:variables] of ESOM or other SOM of same format
Pmatrix	[1:Lines,1:Column] Local densities at each point of the trainedGridWts[1:Lines,1:Column,1:variables] of ESOM or other SOM of same format.

Value

UStarMatrix	[1:Lines,1:Column]
-------------	--------------------

Author(s)

Michael Thrun

References

Ultsch, A. U* C: Self-organized Clustering with Emergent Feature Maps. in Lernen, Wissensentdeckung und Adaptivitaet (LWA). 2005. Saarbruecken, Germany.

Chainlink	<i>Chainlink is part of the Fundamental Clustering Problem Suit (FCPS) [Thrun/Ultsch, 2020].</i>
-----------	--

Description

linear not separable dataset of two intertwined chains.

Usage

```
data("Chainlink")
```

Details

Size 1000, Dimensions 3, stored in Chainlink\$Data

Two clusters, stored in Chainlink\$Cls

Published in [Ultsch et al.,1994] in German and [Ultsch 1995] in English.

References

[Thrun/Ultsch, 2020] Thrun, M. C., & Ultsch, A.: Clustering Benchmark Datasets Exploiting the Fundamental Clustering Problems, Data in Brief, Vol. 30(C), pp. 105501, DOI 10.1016/j.dib.2020.105501, 2020.

[Ultsch 1995] Ultsch, A.: Self organizing neural networks perform different from statistical k-means clustering, Proc. Society for Information and Classification (GFKL), Vol. 1995, Basel 8th-10th March, 1995.

[Ultsch et al.,1994] Ultsch, A., Guimaraes, G., Korus, D., & Li, H.: Knowledge extraction from artificial neural networks and applications, Parallele Datenverarbeitung mit dem Transputer, pp. 148-16Chainlink, Springer, 1994.

Examples

```
data(Chainlink)
str(Chainlink)

## Not run:
require(DataVisualizations)
DataVisualizations::Plot3D(Chainlink$Data,Chainlink$Cls)

## End(Not run)
```

DefaultColorSequence *Default color sequence for plots*

Description

Defines the default color sequence for plots made within the Projections package.

Usage

```
data("DefaultColorSequence")
```

Format

A vector with 562 different strings describing colors for plots.

Delta3DWeightsC *intern function*

Description

The implementation of the main formula of SOM, ESOM, sESOM algorithms.

Usage

Delta3DWeightsC(vx,Datasample)

Arguments

vx Numeric array of weights [1:Lines,1:Columns,1:Weights]
 Datasample Numeric vector of one datapoint[1:n]

Details

intern function in case of ComputeInR==FALSE in [GeneralizedUmatrix](#)

Value

modified array of weights [1:Lines,1:Columns,1:Weights]

Author(s)

Michael Thrun

References

[Thrun, 2018] Thrun, M. C.: Projection Based Clustering through Self-Organization and Swarm Intelligence, doctoral dissertation 2017, Springer, Heidelberg, ISBN: 978-3-658-20539-3, [doi:10.1007/9783658205409](https://doi.org/10.1007/9783658205409), 2018.

EsomNeuronsAsList *Converts wts data (EsomNeurons) into the list form*

Description

Converts wts data into the list form

Arguments

EsomNeurons [1:Lines, 1:Columns, 1:Variables] high dimensional array with grid positions in the first two dimensions.

Details

One could describe this function as a transformation or a special case of wide to long format, see also [ListAsEsomNeurons](#)

Value

TrainedNeurons [1:(Lines*Columns),1:Variables] List of Weights as a matrix (not `list` like in R) as matrix or two dimensional array

Author(s)

Michael Thrun, Florian Lerch

References

Ultsch, A. Maps for the visualization of high-dimensional data spaces. in Proc. Workshop on Self organizing Maps. 2003.

ExtendToroidalUmatrix *Extend Toroidal Umatrix*

Description

Extends Umatrix by toroidal continuation of the given Umatrix defined by ExtendBorders in all four directions.

Usage

```
ExtendToroidalUmatrix(Umatrix, Bestmatches, ExtendBorders)
```

Arguments

Umatrix [1:Lines,1:Columns] Matrix of Umatrix Heights
 Bestmatches [1:n, 1:2] Matrix with positions of Bestmatches for n datapoints, first column is the position in Lines and second column in Columns
 ExtendBorders number of lines and columns the umatrix should be extended with

Details

Function assumes that U-matrix is not planar (has no borders), i.e. is toroidal, and not tiled. Bestmatches are moved to new positions accordingly. Example is shown in conference talk of [Thrun et al., 2020].

Value

Umatrix [1:Lines+2*ExtendBorders,1:Columns+2*ExtendBorders] Matrix of U-Heights
 Bestmatches Array with positions of Bestmatches

Note

Currently can be only used if untiled U-Matrix (the default) is presented, but 4-tiled U-matrix does not work.

Author(s)

Michael Thrun

References

[Thrun et al., 2020] Thrun, M. C., Pape, F., & Ultsch, A.: Interactive Machine Learning Tool for Clustering in Visual Analytics, 7th IEEE International Conference on Data Science and Advanced Analytics (DSAA 2020), Vol. accepted, pp. 1-9, IEEE, Sydney, Australia, 2020.

Examples

#ToDo

GeneralizedUmatrix	<i>Generalized U-Matrix for Projection Methods published in [Thrun/Ultsch, 2020]</i>
--------------------	--

Description

Generalized U-Matrix visualizes high-dimensional distance and density based structures in two-dimensional scatter plots of projection methods like CCA, MDS, PCA or NeRV [Ultsch/Thrun, 2017] with the help of a topographic map with hypsometric tints [Thrun et al. 2016] using a simplified emergent SOM published in [Thrun/Ultsch, 2020].

Usage

```
GeneralizedUmatrix(Data,ProjectedPoints,
PlotIt=FALSE,Cls=NULL,Toroid=TRUE, Tiled=FALSE,
ComputeInR=FALSE,Parallel=FALSE,DataPerEpoch=1,...)
```

Arguments

Data	[1:n,1:d] array of data: n cases in rows, d variables in columns
ProjectedPoints	[1:n,2] matrix containing coordinates of the Projection: A matrix of the fitted configuration.
PlotIt	Optional,bool, default=FALSE, if =TRUE: U-Matrix of every current Position of Databots will be shown However, the amount of details shown will be less than in plotTopographicMap .
Cls	Optional, For plotting, see <code>plotUmatrix</code> in package <code>Umatrix</code>

Toroid	Optional, Default=TRUE, ==FALSE planar computation with borders defined by projection method ==TRUE: toroid borderless (toroidal) computation, the four borders defined by projection method are ignored.
Tiled	Optional, For plotting see <code>plotUmatrix</code> in package <code>Umatrix</code>
ComputeInR	Optional, =T: Rcode, =F Cpp Code
Parallel	Optional, =TRUE: compute parallel Cpp Code, =FALSE do not compute parallel Cpp Code
DataPerEpoch	Optional, scalar, value above zero and below 1 starts sampling and defines percentage of data points sampled in each epoch during the learning phase. Beware: Experimental!
...	Further parameters.

Details

Introduced first in the PhD thesis in [Thrun, 2018, p.46]. Furthermore the two parts of the work were peer-reviewed and published in [Ultsch/Thrun, 2017, Thrun/Ultsch, 2020].

Value

List with	
Umatrix	[1:Lines,1:Columns] Umatrix to be plotted, numerical matrix storing the U-heights, see [Thrun, 2018] for definition.
EsomNeurons	[1:Lines,1:Columns,1:weights] 3-dimensional numeric array (wide format), not wts (long format).
Bestmatches	[1:n,1:2] Positions of GridConverted Projected Points on the Umatrix to the pre-defined Grid by Lines and Columns, First Columns has the content of the Line No and second Column of the Column number.
sESOMparamaters	internals for debugging
Lines	Number of Lines
Columns	Number of Columns
gplotres	output of <code>ggplot2</code>

Author(s)

Michael Thrun

References

[Thrun et al., 2016] Thrun, M. C., Lerch, F., Loetsch, J., & Ultsch, A.: Visualization and 3D Printing of Multivariate Data of Biomarkers, in Skala, V. (Ed.), International Conference in Central Europe on Computer Graphics, Visualization and Computer Vision (WSCG), Vol. 24, Plzen, <http://wscg.zcu.cz/wscg2016/short/A43-full.pdf>, 2016.

[Thrun, 2018] Thrun, M. C.: Projection Based Clustering through Self-Organization and Swarm Intelligence, doctoral dissertation 2017, Springer, Heidelberg, ISBN: 978-3-658-20539-3, doi:10.1007/9783658205409, 2018.

[Ultsch/Thrun, 2017] Ultsch, A., & Thrun, M. C.: Credible Visualizations for Planar Projections, in Cottrell, M. (Ed.), 12th International Workshop on Self-Organizing Maps and Learning Vector Quantization, Clustering and Data Visualization (WSOM), IEEE Xplore, France, 2017.

[Thrun/Ultsch, 2020] Thrun, M. C., & Ultsch, A.: Uncovering High-Dimensional Structures of Projections from Dimensionality Reduction Methods, MethodsX, Vol. in press, pp. 101093. doi 10.1016/j.mex.2020.101093, 2020.

Examples

```
data("Chainlink")
Data=Chainlink$Data
Cls=Chainlink$Cls
InputDistances=as.matrix(dist(Data))
res=cmdscale(d=InputDistances, k = 2, eig = TRUE, add = FALSE, x.ret = FALSE)
ProjectedPoints=as.matrix(res$points)
## Not run:
Stress = ProjectionBasedClustering::KruskalStress(InputDistances,
as.matrix(dist(ProjectedPoints)))

## End(Not run)

resUmatrix=GeneralizedUmatrix(Data,ProjectedPoints)
plotTopographicMap(resUmatrix$Umatrix,resUmatrix$Bestmatches,Cls)
```

GeneratePmatrix

Generates the P-matrix

Description

Generates a P-matrix too visualize only density based structures of high-dimensional data.

Arguments

Data	[1:n,1:d], A [n, d] matrix containing the data
EsomNeurons	[1:Lines,Columns,1:Weights] 3D array of weights given by ESOM or sESOM algorithm.
Radius	The radius for measuring the density within the hypersphere.
PlotIt	If set the Pmatrix will also be plotted
...	If set the Pmatrix will also be plotted

Details

To set the Radius the ABCanalysis of high-dimensional distances can be used [Ultsch/Lötsch, 2015]. For a detailed definition and equation of automated density estimation (Radius) see Thrun et al. 2016.

Value

PMatrix [1:Lines,1:Columns]

Author(s)

Michael Thrun

References

Ultsch, A.: Maps for the visualization of high-dimensional data spaces, Proc. Workshop on Self organizing Maps (WSOM), pp. 225-230, Kyushu, Japan, 2003.

Ultsch, A., Loetsch, J.: Computed ABC Analysis for Rational Selection of Most Informative Variables in Multivariate Data, PloS one, Vol. 10(6), pp. e0129767. doi 10.1371/journal.pone.0129767, 2015.

Thrun, M. C., Lerch, F., Loetsch, J., Ultsch, A.: Visualization and 3D Printing of Multivariate Data of Biomarkers, in Skala, V. (Ed.), International Conference in Central Europe on Computer Graphics, Visualization and Computer Vision,Plzen, 2016.

ListAsEsomNeurons *Converts List to WTS*

Description

Converts wts data in list form into a 3 dimensional array

Arguments

wts_list	[1:(Lines*Columns),1:Variables] Matrix with weights in the 2nd dimension(not list() like in R)
Lines	Lines/Height of the desired grid
Columns	Columns/Width of the desired grid

Details

One could describe this function as a transformation or a special case of long to wide format, see also [EsomNeuronsAsList](#)

Value

EsomNeurons [1:Lines, 1:Columns, 1:Variables] 3 dimensional array containing the weights of the neural grid. For a more general explanation see reference

Author(s)

Michael Thrun, Florian Lerch

References

Ultsch, A.: Maps for the visualization of high-dimensional data spaces, Proc. Workshop on Self organizing Maps (WSOM), pp. 225-230, Kyushu, Japan, 2003.

LowLand

LowLand

Description

LowLand

Usage

LowLand(BestMatchingUnits, GeneralizedUmatrix, Data, Cls, Key, LowLimit)

Arguments

BestMatchingUnits	[1:n,1:n,1:n] BestMatchingUnits =[BMkey, BMLineCoords, BMColCoords]
GeneralizedUmatrix	[1:l,1:c] U-Matrix heights in Matrix form
Data	[1:n,1:d] data cases in lines, variables in Columns or [] or 0
Cls	[1:n] a possible classification of the data or [] or 0
Key	[1:n] the keys of the data or [] or 0
LowLimit	GeneralizedUmatrix heights up to this are considered to lie in the low lands default: LowLimit = prctile(Uheights,80) nur die 80# tiefsten

Value

LowLandBM	the unique BestMatchingUnits in the low lands of an u-Matrix
LowLandInd	index such that UniqueBM = BestMatchingUnits(UniqueInd,)
LowLandData	Data reduced to LowLand: LowLandData = Data(LowLandInd,)
LowLandCls	Cls reduced to LowLand: LowLandCls = Cls(LowLandInd)
LowLandKey	Key reduced to LowLand: LowLandKey = Key(LowLandInd)

Author(s)

ALU 2021 in matlab, MCT reimplemented in R

NormalizeUmatrix	<i>Normalize Umatrix</i>
------------------	--------------------------

Description

Normalizing the U-matrix using the abstract U-Matrix concept [Loetsch/Ultsch, 2014].

Usage

```
NormalizeUmatrix(Data, Umatrix, BestMatches)
```

Arguments

Data	[1:n,1:d] numerical matrix of data with n cases and d variables
Umatrix	[1:lines,1:Columns] matrix of U-heights
BestMatches	[1:n,1:2] Bestmatching units.

Details

see publication [Loetsch/Ultsch, 2014]..

Value

Normalized Umatrix[1:lines,1:Columns] using the abstract U-Matrix concept.

Author(s)

Felix Pape, Michael Thrun

References

Loetsch, J., Ultsch, A.: Exploiting the structures of the U-matrix, in Villmann, T., Schleif, F.-M., Kaden, M. & Lange, M. (eds.), Proc. Advances in Self-Organizing Maps and Learning Vector Quantization, pp. 249-257, Springer International Publishing, Mittweida, Germany, 2014.

Examples

```
data("Chainlink")
Data=Chainlink$Data
Cls=Chainlink$Cls
InputDistances=as.matrix(dist(Data))
res=cmdscale(d=InputDistances, k = 2, eig = TRUE, add = FALSE, x.ret = FALSE)
ProjectedPoints=as.matrix(res$points)
#see also ProjectionBasedClustering package for other common projection methods
```

```
resUmatrix=GeneralizedUmatrix(Data,ProjectedPoints)
## Normalization
```

```

normalizedUmatrix=NormalizeUmatrix(Data,resUmatrix$Umatrix,resUmatrix$Bestmatches)
## visualization
TopviewTopographicMap(GeneralizedUmatrix = normalizedUmatrix,resUmatrix$Bestmatches)

```

plotTopographicMap *Visualizes the Generalized U-matrix in 3D*

Description

The generalized U-matrix is visualized as the topographic map with hypsometric tints. The topographic map represents high-dimensional distance and density-based structures in form of a 3D landscape.

Usage

```

plotTopographicMap(GeneralizedUmatrix, BestMatchingUnits,
  Cls=NULL, ClsColors=NULL, Imx=NULL, Names=NULL,
  BmSize=0.5, RenderingContourLines=TRUE, ...)

```

Arguments

GeneralizedUmatrix	[1:Lines,1:Columns] Umatrix to be plotted, numerical matrix storing the U-heights, see [Thrun, 2018] for definition.
BestMatchingUnits	[1:n,1:2], Positions of bestmatches to be plotted as spheres onto the topographic map
Cls	[1:n], numerical vector of classification of k clusters, one label for each best-match at that given point
ClsColors	Vector of colors that will be used to colorize the different clusters, default is GeneralizedUmatrix::DefaultColorSequence
Imx	a mask (Imx) that will be used to cut out the umatrix
Names	If set: [1:k] character vector naming the k clusters for the legend. In this case, further parameters with the possibility to adjust are: NamesCex: (size); NamesPosition: Legend position; NamesTitle: title of legend; NamesColors: colors if ClsColors are not default (NULL), etc.
BmSize	size(diameter) of the points in the visualizations. The points represent the Best-MatchingUnits
RenderingContourLines	FALSE: disables plotting of contour lines resulting in a much faster plot.

... Besides the legend/names parameter the list of further parameters, use only of you know what you are doing:

Tiled Should the Umatrix be drawn 4times?

ShowAxis shall the axis be shown?

NoLevels number of contour lines

ExtendBorders scalar, extends Umatrix by toroidal continuation of the given Umatrix

Colormap in the case of density p matrix...

title same as main

main same as title

sub same as in [plot](#)

xlab same as in [plot](#)

ylab same as in [plot](#)

zlab same as in [plot](#)

NamesPosition same as in [bgplot3d](#)

NamesColors same as col in [bgplot3d](#)

NamesCex same as cex in [bgplot3d](#)

NamesTitle same as title in [bgplot3d](#)

NamesPch same as pch in [bgplot3d](#)

Details

The visualization of this function is a topographic map with hypsometric tints (Thrun, Lerch, L?tsch, & Ultsch, 2016). "Hypsometric tints are surface colors that represent ranges of elevation (Patterson and Kelso 2004). Here, contour lines are combined with a specific color scale. The color scale is chosen to display various valleys, ridges, and basins: blue colors indicate small distances (sea level), green and brown colors indicate middle distances (low hills), and white colors indicate vast distances (high mountains covered with snow and ice). Valleys and basins represent clusters, and the watersheds of hills and mountains represent the borders between clusters. In this 3D landscape, the borders of the visualization are cyclically connected with a periodicity (L,C). The number of clusters can be estimated by the number of valleys of the visualization. The clustering is valid if mountains do not partition clusters indicated by colored points of the same color and colored regions of points (see examples in section 4.1 and 4.2)."[Thrun/Ultsch, 2020].

A central problem in clustering is the correct estimation of the number of clusters. This is addressed by the topographic map which allows assessing the number of clusters as the number of valleys (Thrun et al., 2016). Please see chapter 5 of [Thrun, 2018] for further details.

Value

An object of class "htmlwidget" in mode invisible, please [rglwidget](#) for details.

Note

First version of algorithm was partly based on the Umatrix package.

Author(s)

Michael Thrun

References

[Thrun, 2018] Thrun, M. C.: Projection Based Clustering through Self-Organization and Swarm Intelligence, doctoral dissertation 2017, Springer, Heidelberg, ISBN: 978-3-658-20539-3, doi:10.1007/9783658205409, 2018.

[Thrun et al., 2016] Thrun, M. C., Lerch, F., Loetsch, J., & Ultsch, A.: Visualization and 3D Printing of Multivariate Data of Biomarkers, in Skala, V. (Ed.), International Conference in Central Europe on Computer Graphics, Visualization and Computer Vision (WSCG), Vol. 24, Plzen, <http://wscg.zcu.cz/wscg2016/short/A43-full.pdf>, 2016.

[Thrun/Ultsch, 2020] Thrun, M. C., & Ultsch, A. : Using Projection based Clustering to Find Distance and Density based Clusters in High-Dimensional Data, Journal of Classification, DOI 10.1007/s00357-020-09373-2, in press, Springer, 2020.

See Also[GeneralizedUmatrix](#)**Examples**

```
data("Chainlink")
Data=Chainlink$Data
Cls=Chainlink$Cls
InputDistances=as.matrix(dist(Data))
res=cmdscale(d=InputDistances, k = 2, eig = TRUE, add = FALSE, x.ret = FALSE)
ProjectedPoints=as.matrix(res$points)
#see also ProjectionBasedClustering package for other common projection methods

resUmatrix=GeneralizedUmatrix(Data,ProjectedPoints)
## visualization
plotTopographicMap(GeneralizedUmatrix = resUmatrix$Umatrix,resUmatrix$Bestmatches)

## Open window in specific resolution
#relevant if Names given

library(rgl)
r3dDefaults$windowRect = c(0,0,1200,1200)
plotTopographicMap(GeneralizedUmatrix = resUmatrix$Umatrix,resUmatrix$Bestmatches)

## Not run:
## To save as STL for 3D printing
  rgl::writeSTL("GenerelizedUmatrix_3d_model.stl")

## Save the visualization as a picture with
library(rgl)
rgl.snapshot('test.png')
```

```

## End(Not run)

## Save interactive html file
## Not run:
widgets=plotTopographicMap(GeneralizedUmatrix = resUmatrix$Umatrix,resUmatrix$Bestmatches)
if(requireNamespace("htmlwidgets"))
  htmlwidgets::saveWidget(widgets,file = "interactiveTopographicMap.html")

## End(Not run)

```

ReduceToLowLand

ReduceToLowLand

Description

ReduceToLowLand

Usage

```
ReduceToLowLand(BestMatchingUnits, GeneralizedUmatrix, Data = NULL, Cls = NULL,
Key = NULL, LowLimit,Force=FALSE)
```

Arguments

BestMatchingUnits	[1:n,1:n,1:n] BestMatchingUnits =[BMkey, BMLineCoords, BMColCoords]
GeneralizedUmatrix	[1:l,1:c] U-Matrix heights in Matrix form
Data	[1:n,1:d] data cases in lines, variables in Columns or [] or 0
Cls	[1:n] a possible classification of the data or [] or 0
Key	[1:n] the keys of the data or [] or 0
LowLimit	GeneralizedUmatrix heights up to this are considered to lie in the low lands default: LowLimit = prctile(Uheights,80) nur die 80# tiefsten
Force	==TRUE: Always perform reduction

Value

LowLandBM	the unique BestMatchingUnits in the low lands of an u-Matrix
LowLandInd	index such that UniqueBM = BestMatchingUnits(UniqueInd,)
LowLandData	Data reduced to LowLand: LowLandData = Data(LowLandInd,)
LowLandCls	Cls reduced to LowLand: LowLandCls = Cls(LowLandInd)
LowLandKey	Key reduced to LowLand: LowLandKey = Key(LowLandInd)

Author(s)

ALU 2021 in matlab, MCT reimplemented in R

sESOM4BMUs

simplified ESOM

Description

internfunction for the simplified ESOM Algorithmus [Thrun/Ultsch, 2020] for fixed BestMatchingUnits

Usage

```
sESOM4BMUs(BMUs,Data, esom, toroid,
CurrentRadius,ComputeInR=FALSE,Parallel=FALSE)
```

Arguments

BMUs	[1:Lines,1:Columns], BestMAatchingUnits generated by ProjectedPoints2Grid()
Data	[1:n,1:d] array of data: n cases in rows, d variables in columns
esom	[1:Lines,1:Columns,1:weights] array of NeuronWeights, see ListAsEsomNeurons()
toroid	TRUE/FALSE - topology of points
CurrentRadius	number between 1 to x
ComputeInR	=T: Rcode, =F Cpp Code
Parallel	=T: Rcode, =F Cpp Code

Details

Algorithm is described in [Thrun, 2018, p. 48, Listing 5.1].

Value

esom	array [1:Lines,1:Columns,1:d], d is the dimension of the weights, the same as in the ESOM algorithm. modified esomneuros regarding a predefined neighborhood defined by a radius
------	--

Note

Usually not for seperated usage!

Author(s)

Michael Thrun

References

[Thrun/Ultsch, 2020] Thrun, M. C., & Ultsch, A.: Uncovering High-Dimensional Structures of Projections from Dimensionality Reduction Methods, MethodsX, Vol. in press, pp. 101093. doi 10.1016/j.mex.2020.101093, 2020.

See Also

[GeneralizedUmatrix](#)

setdiffMatrix	<i>setdiffMatrix shortens Matrix2Curt by those rows that are in both matrices.</i>
---------------	--

Description

setdiffMatrix shortens Matrix2Curt by those rows that are in both matrices.

Arguments

Matrix2Curt	[n,k] matrix, which will be shortened by x rows
Matrix2compare	[m,k] matrix whose rows will be compared to those of Matrix2Curt x rows in Matrix2compare equal rows of Matrix2Curt (order of rows is irrelevant). Has the same number of columns as Matrix2Curt.

Value

V\$CurtedMatrix [n-x,k] Shortened Matrix2Curt

Author(s)

Michael Thrun with the help of Catharina Lippmann

TopviewTopographicMap *Topview of Topographic Map ind 2D*

Description

Fast Visualization of the Generalized U-matrix in 2D which visualizes high-dimensional distance and density based structures of the combination two-dimensional scatter plots (projections) with high-dimensional data.

Usage

```
TopviewTopographicMap(GeneralizedUmatrix, BestMatchingUnits,
  Cls, ClsColors = NULL, Imx = NULL,
  ClsNames = NULL, BmSize = 6, DotLineWidth = 2,
  alpha = 1, ...)
```

Arguments

GeneralizedUmatrix	[1:Lines,1:Columns] Umatrix to be plotted, numerical matrix storing the U-heights, see [Thrun, 2018] for definition.
BestMatchingUnits	[1:n,1:2], Positions of bestmatches to be plotted onto the Umatrix
Cls	[1:n], numerical vector of classification of k classes for the bestmatch at the given point
ClsColors	Vector of colors that will be used to colorize the different classes
Imx	a mask (Imx) that will be used to cut out the umatrix
ClsNames	If set: [1:k] character vector naming the k classes for the legend. In this case, further parameters with the possibility to adjust are: LegendCex: (size); NamesOrientation: Legend position "v" or "h"; NamesTitle: title of legend.
BmSize	size(diameter) of the points in the visualizations. The points represent the Best-MatchingUnits
DotLineWidth	...
alpha	...
...	Tiled Should the Umatrix be drawn 4times? main set specific title in plot ExtendBorders scalar, extends Umatrix by toroidal continuation of the given Umatrix MainCex scalar, magnification to be used for legend LegendCex scalar, magnification to be used for main titles _ Further Arguments relevant for interactive shiny application

Details

Please see [plotTopographicMap](#). This function is currently still experimental because not all functionality is fully tested yet.

Value

plotly handler

Note

Names are currently under development, Imx in testing phase.

Author(s)

Tim Schreier, Luis Winckelmann, Michael Thrun

References

[Thrun, 2018] Thrun, M. C.: Projection Based Clustering through Self-Organization and Swarm Intelligence, doctoral dissertation 2017, Springer, Heidelberg, ISBN: 978-3-658-20539-3, [doi:10.1007/9783658205409](https://doi.org/10.1007/9783658205409), 2018.

[Thrun et al., 2016] Thrun, M. C., Lerch, F., Loetsch, J., & Ultsch, A.: Visualization and 3D Printing of Multivariate Data of Biomarkers, in Skala, V. (Ed.), International Conference in Central Europe on Computer Graphics, Visualization and Computer Vision (WSCG), Vol. 24, Plzen, <http://wscg.zcu.cz/wscg2016/short/A43-full.pdf>, 2016.

See Also

[plotTopographicMap](#)

Examples

```
data("Chainlink")
Data=Chainlink$Data
Cls=Chainlink$Cls
InputDistances=as.matrix(dist(Data))
res=cmdscale(d=InputDistances, k = 2, eig = TRUE, add = FALSE, x.ret = FALSE)
ProjectedPoints=as.matrix(res$points)
#see also ProjectionBasedClustering package for other common projection methods

resUmatrix=GeneralizedUmatrix(Data,ProjectedPoints)
## visualization
TopviewTopographicMap(GeneralizedUmatrix = resUmatrix$Umatrix,resUmatrix$Bestmatches)
```

trainstepC

internal function for s-esom

Description

Does the training for fixed bestmatches in one epoch of the sESOM.

Usage

```
trainstepC(vx,vy, DataSampled,BMUsampled,Lines,Columns, Radius, toroid)
```

Arguments

<code>vx</code>	array [1:Lines,1:Columns,1:Weights], WeightVectors that will be trained, internally transformed von NumericVector to cube
<code>vy</code>	array [1:Lines,1:Columns,1:2], meshgrid for output distance computation
<code>DataSampled</code>	NumericMatrix, n cases shuffled Dataset[1:n,1:d] by sample
<code>BMUsampled</code>	NumericMatrix, n cases shuffled BestMatches[1:n,1:2] by sample in the same way as DataSampled
<code>Lines</code>	double, Height of the grid
<code>Columns</code>	double, Width of the grid
<code>Radius</code>	double, The current Radius that should be used to define neighbours to the bm
<code>toroid</code>	bool, Should the grid be considered with cyclically connected borders?

Details

Algorithm is described in [Thrun, 2018, p. 48, Listing 5.1].

Value

WeightVectors, array[1:Lines,1:Columns,1:weights] with the adjusted Weights

Note

Usually not for seperated usage!

Author(s)

Michael Thrun

References

[Thrun, 2018] Thrun, M. C.: Projection Based Clustering through Self-Organization and Swarm Intelligence, doctoral dissertation 2017, Springer, Heidelberg, ISBN: 978-3-658-20539-3, [doi:10.1007/9783658205409](https://doi.org/10.1007/9783658205409), 2018.

Uheights4Data

Uheights4Data

Description

Uheights4Data

Usage

Uheights4Data(BestMatchingUnits, GeneralizedUmatrix)

Arguments

BestMatchingUnits
 [1:n,1:d] BMKey = BestMatchingUnits[,1]
 GeneralizedUmatrix
 [1:Lines,1:Columns] a GeneralizedUmatrix

Value

Uheights Uheights
 BMLineCoords BMLineCoords
 BMColCoords BMColCoords

Author(s)

ALU 2021 in matlab, MCT reimplemented in

UmatrixColormap	<i>U-Matrix colors</i>
-----------------	------------------------

Description

Defines the default color sequence for plots made for Umatrix

Usage

data("UmatrixColormap")

Format

Returns the vectors for a (heat) colormap.

UniqueBestMatchingUnits	<i>UniqueBestMatchingUnits</i>
-------------------------	--------------------------------

Description

UniqueBestMatchingUnits

Usage

UniqueBestMatchingUnits(NonUniqueBestMatchingUnits)

Arguments

NonUniqueBestMatchingUnits
 [1:n,1:n,1:n] UniqueBestMatchingUnits =[BMkey, BMLineCoords, BMColCoords]

Value

UniqueBM [1:u,1:u,1:u] UniqueBM =[UBMkey, UBMLineCoords, UBMColCoords]
 UniqueInd Index such that UniqueBM = UniqueBestMatchingUnits(UniqueInd,:)
 Uniq2AllInd Index such that UniqueBestMatchingUnits = UniqueBM(Uniq2AllInd,:)

Author(s)

ALU 2021 in matlab, MCT reimplemented in R

upscaleUmatrix *Upscale a Umatrix grid*

Description

Use linear interpolation to increase the size of a umatrix. This can be used to produce nicer ggplot plots in [plotTopographicMap](#) and is going to be used for further normalization of the umatrix.

Usage

```
upscaleUmatrix(Umatrix, Factor = 2, BestMatches, Imx)
```

Arguments

Umatrix The umatrix which should be upscaled
 BestMatches The BestMatches which should be upscaled
 Factor Optional: The factor by which the axes will be scaled. Be aware that the size of the matrix will grow by Factor squared. Default: 2
 Imx Optional: Island cutout of the umatrix. Should also be scaled to the new size of the umatrix.

Value

A List consisting of:

Umatrix A matrix representing the upscaled umatrix.
 BestMatches If BestMatches was given as parameter: The rescaled BestMatches for an island cutout. Otherwise: NULL
 Imx If Imx was given as parameter: The rescaled matrix for an island cutout. Otherwise: NULL

Author(s)

Felix Pape

XYcoords2LinesColumns *XYcoords2LinesColumns(X,Y) Converts points given as x(i),y(i) coordinates to integer coordinates Columns(i),Lines(i)*

Description

XYcoords2LinesColumns(X,Y) Converts points given as x(i),y(i) coordinates to integer coordinates Columns(i),Lines(i)

Arguments

X	[1:n] first coordinate: x(i), y(i) is the i-th point on a plane
Y	[1:n] second coordinate: x(i), y(i) is the i-th point on a plane
minNeurons	minimal size of the corresponding grid i.e $\max(\text{Lines}) * \max(\text{Columns}) \geq \text{MinGridSize}$, default MinGridSize = 4096 defined by the number of neurons
MaxDifferentPoints	TRUE: the discretization error is minimal FALSE: number of Lines and Columns is minimal
PlotIt	Plots the result

Details

Details are written down in [Thrun, 2018, p. 47].

Value

GridConvertedPoints[1:Columns,1:Lines,2] IntegerPositions on a grid corresponding to x,y

Author(s)

Michael Thrun

References

[Thrun, 2018] Thrun, M. C.: Projection Based Clustering through Self-Organization and Swarm Intelligence, doctoral dissertation 2017, Springer, Heidelberg, ISBN: 978-3-658-20539-3, doi:[10.1007/9783658205409](https://doi.org/10.1007/9783658205409), 2018.

Examples

```
data("Chainlink")
Data=Chainlink$Data
InputDistances=as.matrix(dist(Data))
res=cmdscale(d=InputDistances, k = 2, eig = TRUE, add = FALSE, x.ret = FALSE)
ProjectedPoints=as.matrix(res$points)
GridConvertedPoints=XYcoords2LinesColumns(ProjectedPoints[,1],ProjectedPoints[,2],PlotIt=FALSE)
```

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