

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 coercively [Thrun, 2018]. 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 based on the book of Thrun, M.C.: “Projection Based Clustering through Self-Organization and Swarm Intelligence” (2018) <DOI:10.1007/978-3-658-20540-9>.

License GPL-3

Imports Rcpp, ggplot2

Suggests DataVisualizations, DatabionicSwarm, matrixStats, rgl, grid, mgcv, png, ProjectionBasedClustering, reshape2, fields, ABCanalysis, knitr (>= 1.12), rmarkdown (>= 0.9)

LinkingTo Rcpp, RcppArmadillo

Depends R (>= 3.0)

NeedsCompilation yes

SystemRequirements C++11

LazyLoad yes

LazyData TRUE

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

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VignetteBuilder knitr

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

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Alfred Ultsch [ths]

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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]. 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 based on the book of Thrun, M.C.: "Projection Based Clustering through Self-Organization and Swarm Intelligence" (2018) <DOI:10.1007/978-3-658-20540-9>.

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.

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

Index of help topics:

Chainlink	Chainlink is part of the Fundamental Clustering Problem Suit (FCPS) [Ultsch, Chainlink005].
DefaultColorSequence	Default color sequence for plots
Delta3DWeightsC	intern function
GeneralizedUmatrix	Generalized U-Matrix for Projection Methods
GeneralizedUmatrix-package	Credible Visualization for Two-Dimensional Projections of Data
GeneratePmatrix	Generates the P-matrix
UmatrixColormap	U-Matrix colors
XYcoords2LinesColumns	XYcoords2LinesColumns(X,Y) Converts points given as x(i),y(i) coordinates to integer coordinates Columns(i),Lines(i)
plotTopographicMap	Visualizes th Generalized U-matrix
sESOM4BMUs	simplified ESOM
trainstepC	internal function for s-esom
upscaleUmatrix	Upscale a Umatrix grid

Author(s)

Michal Thrun

Maintainer: Michael Thrun <mthrun@informatik.uni-marburg.de>

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, <https://doi.org/10.1007/978-3-658-20540-9>, 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$points)
#see also ProjectionBasedClustering package for other common projection methods
#see DatabionicSwarm for projection method without parameters or objective function
# ProjectedPoints=DatabionicSwarm::Pswarm(Data)$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)

```

Chainlink

*Chainlink is part of the Fundamental Clustering Problem Suit (FCPS)
[Ultsch, Chainlink005].*

Description

linear not separable dataset of two intertwined chains.

Usage

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

Details

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

Teo clusters, stored in Chainlink\$Cls

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

References

Ultsch, A.: Clustering wih SOM: U* C, Proc. Proceedings of the 5th Workshop on Self-Organizing Maps, Vol. Chainlink, pp. 75-8Chainlink, Chainlink005.

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, 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)

library(DataVisualizations)
DataVisualizations::plot3D(Chainlink$Data,Chainlink$CIs)
```

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	array of weights [1:Lines,1:Columns,1:Weights]
Datasample	NumericVector 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, <https://doi.org/10.1007/978-3-658-20540-9>, 2018.

GeneralizedUmatrix *Generalized U-Matrix for Projection Methods*

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 with the help of a topographic map with hypsometric tints [Thrun et al. 2016] based on the Umatrix method for emergent SOMs [Ultsch 2003], for further explanation see [Thrun, 2018]

Usage

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

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=FALSE, ==FALSE planar computation ==TRUE: toroid borderless computation, set so only if projection method is also toroidal
Tiled	Optional, For plotting see <code>plotUmatrix</code> in package <code>Umatrix</code>
ComputeInR	Optional, =T: Rcode, =F Cpp Code

Details

Introduced first in [Thrun, 2018, p.46], additionally reviewed in [Ultsch/Thrun, 2017].

Value

List with	
Umatrix	[1:Lines,1:Columns] (see ReadUMX in package DataIO)
EsomNeurons	[1:Lines,1:Columns,1:weights] 3-dimensional numeric array (wide format), not wts (long format)
Bestmatches	[1:n,OutputDimension] GridConverted Projected Points information converted by convertProjectionProjectedPoints() to predefined Grid by Lines and Columns
gplotres	Ausgabe von ggplot

Author(s)

Michael Thrun

References

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

[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, <https://doi.org/10.1007/978-3-658-20540-9>, 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)
## Not run:
Stress = ProjectionBasedClustering::KruskalStress(InputDistances,

as.matrix(dist(ProjectedPoints)))

## End(Not run)

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

GeneratePmatrix	<i>Generates the P-matrix</i>
-----------------	-------------------------------

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.

plotTopographicMap *Visualizes th Generalized U-matrix*

Description

visualizes high-dimensional distance and density based structures of the combination two-dimensional scatter plots (projections) with high-dimensional data using a topographic map with hypsometric tints.

Usage

```
plotTopographicMap(GeneralizedUmatrix, BestMatchingUnits,
  Cls=NULL, ClsColors=NULL, Imx=NULL, BmSize=0.5, ...)
```

Arguments

GeneralizedUmatrix
(1:Lines,1:Columns), Umatrix to be plotted

BestMatchingUnits
(1:n,1:2), Positions of bestmatches to be plotted onto the Umatrix

Cls
(1:n), Class identifier 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

BmSize
size(diameter) of the points in the visualizations. The points represent the Best-MatchingUnits

...
further parameters, use only if you know what you are doing:

Tiled Should the Umatrix be drawn 4times?

ShowAxis shall the axis be shown?

NoLevels number of contour lines

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](#)

Details

The visualization and result 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 (see (Thrun et al., 2016)). 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 shades of 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). 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 (Thrun et al., 2016). Please see chapter 5 of [Thrun, 2018] for further details.

Note

Algorithm is 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, <https://doi.org/10.1007/978-3-658-20540-9>, 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

[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)
## 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')
```

sESOM4BMUs	<i>simplified ESOM</i>
------------	------------------------

Description

internfunction for the simplified ESOM Algorithmus of [Thrun, 2018] for fixed BestMatchingUnits

Usage

sESOM4BMUs(BMUs,Data, esom, toroid, CurrentRadius,ComputeInR)

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 Codenumber between 1 to x

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, 2018] Thrun, M. C.: Projection Based Clustering through Self-Organization and Swarm Intelligence, doctoral dissertation 2017, Springer, Heidelberg, ISBN: 978-3-658-20539-3, <https://doi.org/10.1007/978-3-658-20540-9>, 2018.

See Also

[GeneralizedUmatrix](#)

trainstepC	<i>internal function for s-esom</i>
------------	-------------------------------------

Description

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

Usage

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

Arguments

vx	array (1:Lines,1:Columns,1:Weights), WeightVectors that will be trained, internally transformed von NumericVector to cube
vy	array (1:Lines,1:Columns,1:2), meshgrid for output distance computation
DataSampled	NumericMatrix, n cases shuffled Dataset[1:n,1:d] by sample
BMUsampled	NumericMatrix, n cases shuffled BestMatches[1:n,1:2] by sample in the same way as DataSampled
Lines	double, Height of the grid
Columns	double, Width of the grid
Radius	double, The current Radius that should be used to define neighbours to the bm
toroid	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, <https://doi.org/10.1007/978-3-658-20540-9>, 2018.

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.

upscaleUmatrix	<i>Upscale a Umatrix grid</i>
----------------	-------------------------------

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), Y(1:n) coordinates: x(i),y(i) is the i-th point on a plane
 minNeurons minimal size of the corresponding grid i.e max(Lines)*max(Columns)>=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, <https://doi.org/10.1007/978-3-658-20540-9>, 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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