## Package 'DatabionicSwarm'

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Type Package License GPL-3

Title Swarm Intelligence for Self-Organized Clustering

Version 2.0.0 Date 2024-06-20

#### Description

Algorithms implementing populations of agents that interact with one another and sense their environment may exhibit emergent behavior such as self-organization and swarm intelligence. Here, a swarm system called Databionic swarm (DBS) is introduced which was published in Thrun, M.C., Ultsch A.: ``Swarm Intelligence for Self-Organized Clustering" (2020), Artificial Intelligence, <DOI:10.1016/j.artint.2020.103237>. DBS is able to adapt itself to structures of high-dimensional data such as natural clusters characterized by distance and/or density based structures in the data space. The first module is the parameterfree projection method called Pswarm (Pswarm()), which exploits the concepts of selforganization and emergence, game theory, swarm intelligence and symmetry considerations. The second module is the parameter-free high-dimensional data visualization technique, which generates projected points on the topographic map with hypsometric tints defined by the generalized U-matrix (GeneratePswarmVisualization()). The third module is the clustering method itself with non-critical parameters (DBSclustering()). Clustering can be verified by the visualization and vice versa. The term DBS refers to the method as a whole. It enables even a non-professional in the field of data mining to apply its algorithms for visualization and/or clustering to data sets with completely different structures drawn from diverse research fields. The comparison to common projection methods can be found in the book of Thrun, M.C.: ``Projection Based Clustering through Self-Organization and Swarm Intelligence" (2018) < DOI:10.1007/978-3-658-20540-9>.

Imports Rcpp (>= 1.0.8), RcppParallel (>= 5.1.4), deldir,
GeneralizedUmatrix, ABCanalysis, ggplot2

**Suggests** DataVisualizations, knitr (>= 1.12), rmarkdown (>= 0.9), plotrix, geometry, sp, spdep, parallel, rgl, png, ProjectionBasedClustering, parallelDist, pracma, dendextend

LinkingTo Rcpp, RcppArmadillo, RcppParallel

**Depends** R (>= 3.0)

**NeedsCompilation** yes

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DatabionicSwarm-package

Swarm Intelligence for Self-Organized Clustering

#### **Description**

Algorithms implementing populations of agents that interact with one another and sense their environment may exhibit emergent behavior such as self-organization and swarm intelligence. Here, a swarm system called Databionic swarm (DBS) is introduced which was published in Thrun, M.C., Ultsch A.: "Swarm Intelligence for Self-Organized Clustering" (2020), Artificial Intelligence, <DOI:10.1016/j.artint.2020.103237>. DBS is able to adapt itself to structures of high-dimensional data such as natural clusters characterized by distance and/or density based structures in the data space. The first module is the parameter-free projection method called Pswarm (Pswarm()), which exploits the concepts of self-organization and emergence, game theory, swarm intelligence and symmetry considerations. The second module is the parameter-free high-dimensional data visualization technique, which generates projected points on the topographic map with hypsometric tints defined by the generalized U-matrix (GeneratePswarmVisualization()). The third module is the clustering method itself with non-critical parameters (DBSclustering()). Clustering can be verified by the visualization and vice versa. The term DBS refers to the method as a whole. It enables even a nonprofessional in the field of data mining to apply its algorithms for visualization and/or clustering to data sets with completely different structures drawn from diverse research fields. The comparison to common projection methods can be found in 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 **DatabionicSwarm** please see the vignette Short Intro to the Databionic Swarm (DBS). The license is CC BY-NC-SA 4.0.

Index of help topics:

DBSclustering Databonic swarm clustering (DBS)

DatabionicSwarm-package

Swarm Intelligence for Self-Organized

Clustering

DefaultColorSequence Default color sequence for plots

Delaunay4Points Adjacency matrix of the delaunay graph for

BestMatches of Points

Delta3DWeightsC intern function, do not use yourself
DijkstraSSSP Internal function: Dijkstra SSSP

GeneratePswarmVisualization

Generates the Umatrix for Pswarm algorithm

Hepta Hepta is part of the Fundamental Clustering

Problem Suit (FCPS) [Thrun/Ultsch, 2020]. Lsun3D Lsun3D is part of the Fundamental Clustering Problem Suit (FCPS) [Thrun/Ultsch, 2020].

Transforms ProjectedPoints to a grid

ProjectedPoints2Grid

Pswarm A Swarm of Databots based on polar coordinates

(Polar Swarm).

PswarmEpochsParallel Intern function, do not use yourself

PswarmEpochsSequential

Intern function, do not use yourself Intern function, do not use yourself

PswarmRadiusParallel PswarmRadiusSequential

intern function, do not use yourself

RelativeDifference Relative Difference

Transforms the Robust Normalization back RobustNorm\_BackTrafo

RobustNormalization RobustNormalization

ShortestGraphPathsC Shortest GraphPaths = geodesic distances

UniquePoints Unique Points

findPossiblePositionsCsingle

Intern function, do not use yourself

getCartesianCoordinates

Intern function: Transformation of Databot

indizes to coordinates

depricated! see GeneralizedUmatrix() getUmatrix4Projection

Generalisierte U-Matrix fuer

Projektionsverfahren

plotSwarm Intern function for plotting during the Pswarm

annealing process

rDistanceToroidCsingle

Intern function for 'Pswarm'

sESOM4BMUs Intern function: Simplified Emergent

Self-Organizing Map

setGridSize Sets the grid size for the Pswarm algorithm

setPolarGrid Intern function: Sets the polar grid

setRmin Intern function: Estimates the minimal radius

for the Databot scent

setdiffMatrix setdiffMatrix shortens Matrix2Curt by those

rows that are in both matrices.

internal function for s-esom trainstepC trainstepC2 internal function for s-esom

#### Note

For interactive Island Generation of a generalized Umatrix see interactiveGeneralizedUmatrixIsland function in the package ProjectionBasedClustering.

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

#### Author(s)

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Maintainer: Michael Thrun <m.thrun@gmx.net>

#### References

[Thrun/Ultsch, 2021] Thrun, M. C., and Ultsch, A.: Swarm Intelligence for Self-Organized Clustering, Artificial Intelligence, Vol. 290, pp. 103237, doi:10.1016/j.artint.2020.103237, 2021.

[Thrun/Ultsch, 2021] Thrun, M. C., & Ultsch, A.: Swarm Intelligence for Self-Organized Clustering (Extended Abstract), in Bessiere, C. (Ed.), 29th International Joint Conference on Artificial Intelligence (IJCAI), Vol. IJCAI-20, pp. 5125–5129, doi:10.24963/ijcai.2020/720, Yokohama, Japan, Jan., 2021.

[Thrun/Ultsch, 2020] Thrun, M. C., & Ultsch, A.: Uncovering High-Dimensional Structures of Projections from Dimensionality Reduction Methods, MethodsX, Vol. 7, pp. 101093, DOI 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.

[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.

Successfully used in

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[Weyer-Menkhoff et al., 2018] Weyer-Menkhoff, I., Thrun, M. C., & Loetsch, J.: Machine-learned analysis of quantitative sensory testing responses to noxious cold stimulation in healthy subjects, European Journal of Pain, Vol. 22(5), pp. 862-874, DOI doi:10.1002/ejp.1173, 2018.

[Kringel et al., 2018] Kringel, D., Geisslinger, G., Resch, E., Oertel, B. G., Thrun, M. C., Heinemann, S., & Loetsch, J.: Machine-learned analysis of the association of next-generation sequencing based human TRPV1 and TRPA1 genotypes with the sensitivity to heat stimuli and topically applied capsaicin, Pain, Vol. 159 (7), pp. 1366-1381, DOI doi:10.1097/j.pain.00000000000001222, 2018

[Thrun, 2019] Thrun, M. C.: Cluster Analysis of Per Capita Gross Domestic Products, Entrepreneurial Business and Economics Review (EBER), Vol. 7(1), pp. 217-231, DOI: doi:10.15678/EBER.2019.070113, 2019.

[Lopez-Garcia et al., 2020] Lopez-Garcia, P., Argote, D. L., & Thrun, M. C.: Projection-based Classification of Chemical Groups and Provenance Analysis of Archaeological Materials, IEEE Access, Vol. 8, pp. 152439-152451, DOI doi:10.1109/ACCESS.2020.3016244, 2020.

#### **Examples**

```
data('Lsun3D')
##2d projection, without instant visualization of steps
#Alternative I:
#DistanceMatrix hast to be defined by the user.
InputDistances=as.matrix(dist(Lsun3D$Data))
projection=Pswarm(InputDistances)
#2d projection, with instant visualization
## Not run:
#Alternative II: DataMatrix, Distance is Euclidean per default
projection=Pswarm(Lsun3D$Data,Cls=Lsun3D$Cls,PlotIt=T)
## End(Not run)
##Computation of Generalized Umatrix
# If Non Euclidean Distances are used, Please Use \code{MDS}
# from the ProjectionBasedClustering package with the correct OutputDimension
# to generate a new DataMatrix from the distances (see SheppardDiagram
# or KruskalStress)
genUmatrixList=GeneratePswarmVisualization(Data = Lsun3D$Data,
projection$ProjectedPoints,projection$LC)
## Visualizuation of GenerelizedUmatrix,
# Estimation of the Number of Clusters=Number of valleys
library(GeneralizedUmatrix)#install if not installed
GeneralizedUmatrix::plotTopographicMap(genUmatrixList$Umatrix,genUmatrixList$Bestmatches)
## Automatic Clustering
# number of Cluster from dendrogram (PlotIt=TRUE) or visualization
Cls=DBSclustering(k=3, Lsun3D$Data, genUmatrixList$Bestmatches,
genUmatrixList$LC,PlotIt=FALSE)
# Verification, often its better to mark Outliers manually
GeneralizedUmatrix::plotTopographicMap(genUmatrixList$Umatrix,genUmatrixList$Bestmatches,Cls)
## Not run:
# To generate the 3D landscape in the shape of an island
# from the toroidal topograpic map visualization
# you may cut your island interactivly around high mountain ranges
Imx = ProjectionBasedClustering::interactiveGeneralizedUmatrixIsland(genUmatrixList$Umatrix,
genUmatrixList$Bestmatches,Cls)
GeneralizedUmatrix::plotTopographicMap(genUmatrixList$Umatrix,
genUmatrixList$Bestmatches, Cls=Cls,Imx = Imx)
## End(Not run)
## Not run:
library(ProjectionBasedClustering)#install if not installed
Cls2=ProjectionBasedClustering::interactiveClustering(genUmatrixList$Umatrix,
genUmatrixList$Bestmatches, Cls)
```

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## End(Not run)

DBSclustering Databonic swarm clustering (DBS)

## **Description**

DBS is a flexible and robust clustering framework that consists of three independent modules. The first module is the parameter-free projection method Pswarm Pswarm, which exploits the concepts of self-organization and emergence, game theory, swarm intelligence and symmetry considerations [Thrun/Ultsch, 2021]. The second module is a parameter-free high-dimensional data visualization technique, which generates projected points on a topographic map with hypsometric colors GeneratePswarmVisualization, called the generalized U-matrix. The third module is a clustering method with no sensitive parameters DBSclustering (see [Thrun, 2018, p. 104 ff]). The clustering can be verified by the visualization and vice versa. The term DBS refers to the method as a whole.

The DBSclustering function applies the automated Clustering approach of the Databonic swarm using abstract U distances, which are the geodesic distances based on high-dimensional distances combined with low dimensional graph paths by using ShortestGraphPathsC.

#### Usage

```
DBSclustering(k, DataOrDistance, BestMatches, LC, StructureType = TRUE,
PlotIt = FALSE, ylab,main, method = "euclidean",...)
```

## **Arguments**

k	number of clusters, how many to you see in the topographic map (3D land-scape)?
DataOrDistance	Either [1:n,1:d] Matrix of Data (n cases, d dimensions) that will be used. One DataPoint per row or symmetric Distance matrix [1:n,1:n]
BestMatches	[1:n,1:2] Matrix with positions of Bestmatches or ProjectedPoints, one matrix line per data point
LC	grid size c(Lines, Columns), please see details
StructureType	Optional, bool; = TRUE: compact structure of clusters assumed, =FALSE: connected structure of clusters assumed. For the two options for Clusters, see [Thrun, 2018] or Handl et al. 2006
PlotIt	Optional, bool, Plots Dendrogramm
ylab	Optional, character vector, ylabel of dendrogramm
main	Optional, character vctor, title of dendrogramm
method	Optional, one of 39 distance methods of parDist of package parallelDist, if Data matrix is chosen above
•••	Further arguments passed on to the parDist function, e.g. user-defined distance functions

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#### **Details**

The input of the LC parameter depends on the choice of Bestmatches input argument. Usually as the name of the argument states, the Bestmatches of the GeneratePswarmVisualization function are used which is define in the notation of self-organizing map. In this case please see example one.

However, as written above, clustering and visualization can be applied independently of each other. In this case the places of Lines L and Columns C are switched because Lines is a value slightly above the maximum of the x-coordinates and Columns is a value slightly above the maximum of the y-coordinates of ProjectedPoint. Hence, one should give DBSclustering the argument LC as shown in example 2.

Often it is better to mark the outliers manually after the prozess of clustering and sometimes a clustering can be improved through human interaction [Thrun/Ultsch,2017] <DOI:10.13140/RG.2.2.13124.53124>; use in this case the visualization plotTopographicMap of the package GeneralizedUmatrix. If you would like to mark the outliers interactivly in the visualization use the **ProjectionBasedClustering** package with the function interactiveClustering(), or for full interactive clustering IPBC(). The package is available on CRAN. An example is shown in case of interactiveClustering() function in the third example.

#### Value

[1:n] numerical vector of numbers defining the classification as the main output of this cluster analysis for the n cases of data corresponding to the n bestmatches. It has k unique numbers representing the arbitrary labels of the clustering. You can use plotTopographicMap(Umatrix, Bestmatches, Cls) for verification.

#### Note

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

#### Author(s)

Michael Thrun

## References

[Thrun/Ultsch, 2021] Thrun, M. C., and Ultsch, A.: Swarm Intelligence for Self-Organized Clustering, Artificial Intelligence, Vol. 290, pp. 103237, doi:10.1016/j.artint.2020.103237, 2021.

## **Examples**

```
data("Lsun3D")
Data=Lsun3D$Data
InputDistances=as.matrix(dist(Data))
projection=Pswarm(InputDistances)
## Example One
genUmatrixList=GeneratePswarmVisualization(Data,
```

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```
projection$ProjectedPoints,projection$LC)
Cls=DBSclustering(k=3, Data, genUmatrixList$Bestmatches,
genUmatrixList$LC,PlotIt=TRUE)
## Example Two
#automatic Clustering without GeneralizedUmatrix visualization
Cls=DBSclustering(k=3, Data, projection$ProjectedPoints,projection$LC,
PlotIt=TRUE)
## Not run:
## Example Three
## Sometimes an automatic Clustering can be improved
## through an interactive approach,
## e.g. if Outliers exist (see [Thrun/Ultsch, 2017])
library(ProjectionBasedClustering)
{\tt Cls2=ProjectionBasedClustering::interactiveClustering(genUmatrixList\$Umatrix,}
genUmatrixList$Bestmatches, 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.

Delaunay4Points

Adjacency matrix of the delaunay graph for BestMatches of Points

#### Description

Calculates the adjacency matrix of the delaunay graph for BestMatches (BMs) in tiled form if BestMatches are located on a toroid grid

#### Usage

```
Delaunay4Points(Points, IsToroid = TRUE,LC,PlotIt=FALSE,Gabriel=FALSE)
```

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## **Arguments**

Points [1:n,1:3] matrix containing the BMKey, X and Y coordinates of the n, Best-

Matches NEED NOT to be UNIQUE, however, there is an edge in the Deaunay

between duplicate points!

IsToroid Optional, logical, indicating if BM's are on a toroid grid. Default is True

LC Optional, A vector of length 2, containing the number of lines and columns of

the Grid

PlotIt Optional, bool, Plots the graph

Gabriel Optional, bool, default: FALSE, If TRUE: calculates the gabriel graph instead

of the delaunay graph

#### Value

Delaunay[1:n,1:n] adjacency matrix of the Delaunay-Graph

#### 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.

Delta3DWeightsC

intern function, do not use yourself

## Description

Delta3DWeightsC

## Usage

Delta3DWeightsC(vx, Datasample)

## **Arguments**

vx Array [1:n,1:m,1:d] of neuron weights on a nxm grid with d dimensional weights.

Datasample One observation of a d-dimensional datapoint.

## **Details**

Algorithm is described in [Thrun, 2018, p. 95, Listing 8.1].

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#### Value

vx Array [1:n,1:m,1:1]

#### 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.

DijkstraSSSP Internal function: Dijkstra SSSP

## Description

Dijkstra's SSSP (Single source shortest path) algorithm:

gets the shortest path (geodesic distance) from source vertice(point) to all other vertices(points) defined by the edges of the adjasency matrix

#### Usage

```
DijkstraSSSP(Adj, Costs, source)
```

#### **Arguments**

Adj [1:n,1:n] 0/1 adjascency matrix, e.g. from delaunay graph or gabriel graph

Costs [1:n,1:n] matrix, distances between n points (normally euclidean)

source int, vertice(point) from which to calculate the geodesic distance to all other

points

#### **Details**

Preallocating space for DataStructures accordingly to the maximum possible number of vertices which is fixed set at the number 10001. This is an internal function of ShortestGraphPathsC, no errors or mis-usage is caught here.

#### Value

ShortestPaths[1:n] vector, shortest paths (geodesic) to all other vertices including the source vertice itself

#### Note

runs in O(E\*Log(V))

#### Author(s)

Michael Thrun

#### References

uses a changed code which is inspired by Shreyans Sheth 28.05.2015, see <a href="https://ideone.com/qkmt31">https://ideone.com/qkmt31</a>

findPossiblePositionsCsingle

Intern function, do not use yourself

## **Description**

Finds all possible jumping position regarding a grid and Radius for DataBots

#### **Usage**

```
findPossiblePositionsCsingle(RadiusPositionsschablone,
  jumplength, alpha, Lines)
```

#### **Arguments**

RadiusPositionsschablone

NumericMatrix, see setPolarGrid

jumplength double radius of databots regarding neighborhood, they can jump to

alpha double, zu streichen

Lines double, jumpinglength has to smaller than Lines/2 and Lines/2 has to yield to a

integer number.

#### **Details**

Algorithm is described in [Thrun, 2018, p. 95, Listing 8.1].

## Value

OpenPositions NumericMatrix, indizes of open positions

## 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.

#### See Also

setPolarGrid

GeneratePswarmVisualization

Generates the Umatrix for Pswarm algorithm

#### **Description**

DBS is a flexible and robust clustering framework that consists of three independent modules. The first module is the parameter-free projection method Pswarm Pswarm, which exploits the concepts of self-organization and emergence, game theory, swarm intelligence and symmetry considerations. The second module is a parameter-free high-dimensional data visualization technique, which generates projected points on a topographic map with hypsometric colors GeneratePswarmVisualization, called the generalized U-matrix. The third module is a clustering method with no sensitive parameters DBSclustering. The clustering can be verified by the visualization and vice versa. The term DBS refers to the method as a whole.

The GeneratePswarmVisualization function generates the special case (please see [Thrun, 2018]) of the generalized Umatrix with the help of an unsupervised neural network (simplified emergent self-organizing map published in [Thrun/Ultsch, 2020]). From the generalized Umatrix a topographic map with hypsometric tints can be visualized. To see this visualization use plotTopographicMap of the package GeneralizedUmatrix.

#### Usage

```
GeneratePswarmVisualization(Data, ProjectedPoints, LC, PlotIt=FALSE,
ComputeInR=FALSE, Parallel=TRUE, Tiled = FALSE, DataPerEpoch = 1)
```

## **Arguments**

Data [1:n,1:d] array of data: n cases in rows, d variables in columns

ProjectedPoints

matrix, ProjectedPoints[1:n,1:2] n by 2 matrix containing coordinates of the Projection: A matrix of the fitted configuration. see output of Pswarm for further

details

LC size of the grid c(Lines, Columns), number of Lines and Columns automatic

calculated by setGridSize in Pswarm

Sometimes is better to choose a different grid size, e.g. to to reduce computional effort contrary to SOM, here the grid size defined only the resolution of the visualizations The real grid size is predfined by Pswarm, but you may choose a factor x\*res\$LC if you so desire. Therefore, The resulting grid size is given

back in the Output.

PlotIt Optional, default(FALSE), If TRUE than uses plotTopographicMap of the pack-

age GeneralizedUmatrix is plotted as a topview in the tiled option, see details

for explanation.

ComputeInR Optional, =TRUE: Rcode, =FALSE C++ implementation

Parallel Optional, =TRUE: Parallel C++ implementation, =FALSE Sequential C++ im-

plementation

Tiled Optional, =TRUE: arrangement of four grids for better understanding of edge

behaviour, =FALSE: single grid.

DataPerEpoch Optional: Number between 0 and 1 stating the ratio of data per epoch for training

of the generalized u-matrix approach.

#### **Details**

Tiled: The topographic map is visualized 4 times because the projection is toroidal. The reason is that there are no border in the visualizations and clusters (if they exist) are not disrupted by borders of the plot.

If you used Pswarm with distance matrix instead of a data matrix (in the sense that you do not have any data matrix available), you may transform your distances into data by using MDS of the **ProjectionBasedClustering** package in order to use the GeneratePswarmVisualization function. The correct dimension can be found through the Sheppard diagram or kruskals stress.

#### Value

list of

Bestmatches matrix [1:n,1:2], BestMatches of the Umatrix, contrary to ESOM they are al-

ways fixed, because predefined by GridPoints.

Umatrix matrix [1:Lines,1:Columns],

WeightsOfNeurons

array [1:Lines,1:Columns,1:d], d is the dimension of the weights, the same as in

the ESOM algorithm

GridPoints matrix [1:n,1:2], quantized projected points: projected points now lie on a pre-

defined grid.

LC c(Lines, Columns), normally equal to grid size of Pswarm, sometimes it a better

or a lower resolution for the visualization is better. Therefore here the grid size

of the neurons is given back.

PlotlyHandle If PlotIt=FALSE: NULL, otherwise plotly object for ploting topview of topo-

graphic map

#### Note

If you used pswarm with distance matrix instead of a data matrix you can mds transform your distances into data (see the MDS function of the ProjectionBasedClustering package.). The correct dimension can be found through the Sheppard diagram or kruskals stress.

#### Note

The extraction of an island out of the generalized Umatrix can be performed using the interactiveGeneralizedUmatrixIsI function in the package **ProjectionBasedClustering**.

The main code of both functions GeneralizedUmatrix and GeneratePswarmVisualization is the same C++ function sESOM4BMUs which is described in [Thrun/Ultsch, 2020].

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#### 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/Ultsch, 2020] Thrun, M. C., & Ultsch, A.: Uncovering High-Dimensional Structures of Projections from Dimensionality Reduction Methods, MethodsX, Vol. 7, pp. 101093, doi:10.1016/j.mex.2020.101093, 2020.

#### See Also

Pswarm and plotTopographicMap and GeneralizedUmatrix of the package GeneralizedUmatrix

#### **Examples**

```
data("Lsun3D")
Data=Lsun3D$Data
Cls=Lsun3D$Cls
InputDistances=as.matrix(dist(Data))

projList=Pswarm(InputDistances)
genUmatrixList=GeneratePswarmVisualization(Data,projList$ProjectedPoints,projList$LC)
library(GeneralizedUmatrix)
plotTopographicMap(genUmatrixList$Umatrix,genUmatrixList$Bestmatches,Cls)
```

 ${\tt getCartesianCoordinates}$ 

Intern function: Transformation of Databot indizes to coordinates

## Description

Transforms Databot indizes to exact cartesian coordinates on an toroid two dimensional grid.

## Usage

```
getCartesianCoordinates(DataBotsPosRe, DataBotsPosIm, GridRadius, GridAngle,
QuadOrHexa = TRUE)
```

#### Arguments

DataBotsPosRe [1:N] real part of complex vector Two Indizes per Databot describing its posi-

tions in an two dimensional grid

DataBotsPosIm [1:N] imaginary part of complex vector Two Indizes per Databot describing its

positions in an two dimensional grid

GridRadius [Columns, Lines] Radii Matrix of all possible Positions of DataBots in Grid, see

also documentation of setPolarGrid

GridAngle [Columns, Lines] Angle Matrix of all possible Positions of DataBots in Grid,

see also documentation of setPolarGrid

QuadOrHexa Optional, FALSE=If DataPos on hexadiagonal grid, round to 2 decimals after

value, Default=TRUE

#### **Details**

Transformation is described in [Thrun, 2018, p. 93].

#### Value

 ${\tt BestMatchingUnits}$ 

[1:N,2] coordinates on an two dimensional grid for each databot excluding unique key, such that by using GeneratePswarmVisualization a visualization of the Pswarm projection is possible

#### 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.

 $\label{lem:getUmatrix4Projection} \textit{depricated! see GeneralizedUmatrix() Generalisierte $U$-Matrix fuer} \\ \textit{Projektionsverfahren}$ 

## **Description**

depricated! see GeneralizedUmatrix()

## Usage

```
getUmatrix4Projection(Data,ProjectedPoints,
PlotIt=TRUE,Cls=NULL,toroid=T,Tiled=F,ComputeInR=F)
```

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#### Arguments

Data [1:n,1:d] array of data: n cases in rows, d variables in columns

ProjectedPoints

[1:n,2]n by 2 matrix containing coordinates of the Projection: A matrix of the

fitted configuration.

PlotIt Optional, bool, defaut=FALSE, if =TRUE: U-Marix of every current Position of

Databots will be shown

Cls Optional, For plotting, see plotUmatrix in package Umatrix

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 plotUmatrix in package Umatrix

ComputeInR Optional, =T: Rcode, =F Cpp Code

#### Value

List with

Umatrix [1:Lines,1:Columns] (see ReadUMX in package DataIO)

EsomNeurons [Lines, Columns, 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

unbesetztePositionen

Umatrix[unbesetztePositionen] =NA

## Author(s)

Michael Thrun

#### References

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

#### **Examples**

```
data("Lsun3D")
Data=Lsun3D$Data
Cls=Lsun3D$Cls
InputDistances=as.matrix(dist(Data))
res=cmdscale(d=InputDistances, k = 2, eig = TRUE, add = FALSE, x.ret = FALSE)
ProjectedPoints=as.matrix(res$points)
# Stress = KruskalStress(InputDistances, as.matrix(dist(ProjectedPoints)))
#resUmatrix=GeneralizedUmatrix(Data,ProjectedPoints)
#plotTopographicMap(resUmatrix$Umatrix,resUmatrix$Bestmatches,Cls)
```

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Hepta	Hepta is part of the Fundamental Clustering Problem Suit (FCPS) [Thrun/Ultsch, 2020].

## **Description**

clearly defined clusters, different variances

## Usage

```
data("Hepta")
```

## **Details**

Size 212, Dimensions 3, stored in Hepta\$Data Classes 7, stored in Hepta\$Cls

#### 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.

## **Examples**

```
data(Hepta)
str(Hepta)
```

Lsun3D

Lsun3D is part of the Fundamental Clustering Problem Suit (FCPS) [Thrun/Ultsch, 2020].

## Description

clearly defined clusters, different variances

#### Usage

```
data("Lsun3D")
```

#### **Details**

Size 404, Dimensions 3

Dataset defined discontinuites, where the clusters have different variances. Three main Clusters, and four Outliers (in Cluster 4). See for a more detailed description in [Thrun, 2018].

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#### 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.

## **Examples**

data(Lsun3D)
str(Lsun3D)
Cls=Lsun3D\$Cls
Data=Lsun3D\$Data

plotSwarm

Intern function for plotting during the Pswarm annealing process

## Description

Intern function, generates a scatter plot of the progess of the Pswarm algorithm after every nash equlibirum. Every point symbolizes a Databot. If a prior classification is given (Cls) then the Databots have the colors defined by the class labels.

## Usage

```
plotSwarm(Points,Cls,xlab,ylab,main)
```

## **Arguments**

Points	ProjectedPoints or DataBot positions in cartesian coordinates
Cls	optional, Classification as a numeric vector, if given
xlab	='X', optional, string
ylab	='Y', optional, string
main	="DataBots", optional, string

#### Author(s)

Michael Thrun

## See Also

Pswarm with PlotIt=TRUE

20 ProjectedPoints2Grid

ProjectedPoints2Grid Transforms ProjectedPoints to a grid

#### **Description**

quantized xy cartesianncoordinates of ProjectedPoints

#### Usage

ProjectedPoints2Grid(ProjectedPoints, Lines, Columns, PlotIt=FALSE, Cls)

## **Arguments**

ProjectedPoints

[1:n,1:2] matrix of cartesian xy coordinates

Lines double, length of small side of the rectangular grid
Columns double, length of big side of the rectangular grid

PlotIt optional, bool, shows the result if TRUE

Cls Numeric vector containing the classification vector.

#### **Details**

intern function, described in [Thrun, 2018, p.47]

#### Value

BestMatches[1:n,1:3] columns in order: Key,Lines,Columns

#### 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.

#### See Also

GeneratePswarmVisualization

Pswarm 21

Pswarm	A Swarm of Databots based on polar coordinates (Polar Swarm).
	•

## Description

This projetion method is a part of the databionic swarm which uses the nash equlibrium [Thrun/Ultsch, 2021]. Using polar coordinates for agents (here Databots) in two dimensions has many advantages, for further details see [Thrun, 2018] and [Thrun/Ultsch, 2021].

## Usage

```
Pswarm(DataOrDistance, Cls = NULL, QuadOrHexa = "Hexa", NumJumps = 4,
LC = NULL, Parallel = FALSE, NCores = "max", Verbose = 1,
PlotIt = FALSE, Debug = FALSE, DistanceMeasure = "euclidean",
Eps = 0.001)
```

## Arguments

Eps

DataOrDistance	Numeric matrix nxd. Two cases here: $d=n \Rightarrow$ assuming distance matrix $d!=n \Rightarrow$ assuming data matrix with n cases and d features implying the need to compute the distance matrix internally.
Cls	Numeric vector [1:n] with class labels for each observation in DataOrDistance.
QuadOrHexa	Optional, Boolean indicating the geometry of tiles the 2D projection plane is built with.
NumJumps	Integer indicating the number of jumps to be considered for each single databot selected for jumping.
LC	Optional, grid size $c(Columns, Lines)$ , sometimes it is better to call ${\tt setGridSize}$ separately.
Parallel	Optional, Boolean: TRUE = parallel execution, FALSE = single thread execution.
NCores	Character or integer: choice of number of cores of CPU (in case). Can be 'max' or a number. The max will always be 'all available cores - 1', to avoid core overload.
PlotIt	Optional, bool, default=FALSE, If =TRUE, Plots the projection during the computation prozess after every nash equlibirum.
Debug	Optional, Debug, default=FALSE, =TRUE results in various console messages, depricated for CRAN, because cout is not allowed.
DistanceMeasure	e
	Optional, one of 39 distance methods of parDist of package parallelDist, if Data matrix is chosen above
Verbose	optional, integer stating the degree of textual feedback. $0 = \text{no}$ output, $1 = \text{basic}$ notifications, $2 = \text{progress bar}$ , $3 = \text{details}$ .

optional, double: Stop criterion for convergence of each epoche.

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#### **Details**

DBS is a flexible and robust clustering framework that consists of three independent modules. The first module is the parameter-free projection method Pswarm Pswarm, which exploits the concepts of self-organization and emergence, game theory, swarm intelligence and symmetry considerations. The second module is a parameter-free high-dimensional data visualization technique, which generates projected points on a topographic map with hypsometric colors <code>GeneratePswarmVisualization</code>, called the generalized U-matrix. The third module is a clustering method with no sensitive parameters <code>DBSclustering</code>. The clustering can be verified by the visualization and vice versa. The term <code>DBS</code> refers to the method as a whole.

#### Value

List with

ProjectedPoints

[1:n,1:2] xy cartesian coordinates of projection

LC number of Lines and Columns in c(Lines, Columns)

Control List, only for intern debugging

#### Note

LC is now automatically estimated; LC is the size of the grid c(Lines, Columns), number of Lines and Columns, default c(NULL,NULL) and automatic calculation by setGridSize.

#### Author(s)

Michael Thrun, Quirin Stier

#### 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/Ultsch, 2021] Thrun, M. C., and Ultsch, A.: Swarm Intelligence for Self-Organized Clustering, Artificial Intelligence, Vol. 290, pp. 103237, doi:10.1016/j.artint.2020.103237, 2021.

[Stier/Thrun, 2024] Stier, Q. and Thrun, M. C.: An efficient multicore CPU implementation of the DatabionicSwarm, 18th conference of the International Federation of Classification Societies (IFCS), San José, Costa Rica, July 14-19, 2024.

#### **Examples**

```
data("Lsun3D")
Data=Lsun3D$Data
Cls=Lsun3D$Cls
InputDistances=as.matrix(dist(Data))
#If not called separately setGridSize() is called in Pswarm
LC=setGridSize(InputDistances)
res=Pswarm(InputDistances,LC=LC,Cls=Cls,PlotIt=TRUE)
```

PswarmEpochsParallel Intern function, do not use yourself

#### **Description**

Finds the weak Nash equilibrium of the data bots for one epoch depending on a radius, which requires the setting of constants, grid, and so on in, see Pswarm.

#### **Usage**

PswarmEpochsParallel(AllDataBotsPosRe, AllDataBotsPosIm, MyDistanceMatrix, AllFreePosR0, GridRadii, GridAngle, JumpsPerRadius, NumJumps, NumAllDB, Lines, Columns, Origin, Happiness, QuadOrHexa, RadiusVector, Rmin, Rmax, Cls, Debug, pp, PlotIt = FALSE, Verbose = 1, Eps = 0.0001)

## **Arguments**

AllDataBotsPosRe

Numeric vector [1:n] of the current positions for the databots on first of two dimensions.

AllDataBotsPosIm

Numeric vector [1:n] of the current positions for the databots on second of two dimensions.

MyDistanceMatrix

Numeric vector with vectorized distance matrix of the datapoints in the original

(high-dimensional) data space

AllFreePosR0 NumericMatrix, see AllallowedDBPosR0 in setPolarGrid

GridRadii Numeric matrix with radius information of polar transformation for each grid

position

GridAngle Numeric matrix with angle information of polar transformation for each grid

position

JumpsPerRadius Numeric Vector of possible positions of the 1st coordinate.

NumJumps Integer number of jumps.

NumAllDB Integer total number of databots

Lines Integer stating the number of Lines the polar grid consists of.

Columns Integer stating the number of columns the polar grid consists of.

Origin Numeric origin of the positions of grid in two dimensions

Happiness Numeric value indicating the global happiness over all databots

QuadOrHexa optional, bool: If TRUE prints status every 100 iterations

RadiusVector Numeric vector stating all moving radius in a descending order (cooling down

scheme).

Rmin Integer stating minimum radius.

Rmax Integer stating maximum radius.

Cls Integer vector stating the classification vector for each datapoints/databots.

Debug optional, bool: If TRUE prints information for debugging.

pp Numeric vector stating ratio of number of jumping simultaneously DataBots

of one eppoch (per nash-equilibirum), this vector is linearly monotonically de-

creasing.

PlotIt optional, bool: If TRUE creates plot of projection after each epoch.

Verbose optional, integer stating degree of textual feedback. 0 = no output, 1 = basic

notifications, 2 = progress bar, 3 = details.

Eps optional, double: Stop criterion for convergence of each epoche.

#### **Details**

Algorithm is described in [Thrun, 2018, p. 95, Listing 8.1].

#### Value

list of

AllDataBotsPosRe

Numeric vector [1:n] of the current positions for the databots on first of two dimensions.

AllDataBotsPosIm

Numeric vector [1:n] of the current positions for the databots on second of two dimensions.

CourseOfHappiness

Numeric Vector, states the global happiness value per epoch.

RadiusPerEpoch NumericVector, stating the radius used per epoch in order of computation.

#### Author(s)

Quirin Stier

#### 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/Ultsch, 2021] Thrun, M. C., and Ultsch, A.: Swarm Intelligence for Self-Organized Clustering, Artificial Intelligence, Vol. 290, pp. 103237, doi:10.1016/j.artint.2020.103237, 2021.

[Stier/Thrun, 2024] Stier, Q. and Thrun, M. C.: An efficient multicore CPU implementation of the DatabionicSwarm, 18th conference of the International Federation of Classification Societies (IFCS), San José, Costa Rica, July 14-19, 2024.

## PswarmEpochsSequential

Intern function, do not use yourself

#### **Description**

Finds the weak Nash equilibirium of the data bots for one epoch depending on a radius, which requires the setting of constants, grid, and so on in, see Pswarm.

#### Usage

```
PswarmEpochsSequential(AllDataBotsPos, MyDistanceMatrix, IndPossibleDBPosR, AllFreePosR0, NumAllDB, Lines, Columns, Origin, Happiness, GridRadii, GridAngle, QuadOrHexa, RadiusVector, Rmin, Rmax, Cls, Debug, pp, PlotIt = FALSE, Verbose = 1)
```

## **Arguments**

AllDataBotsPos Complex vector [1:n] of the current positions for the databots on a 2d and real plane in complex numbers.

MyDistanceMatrix

Numeric vector with vectorized distance matrix of the datapoints in the original (high-dimensional) data space

 ${\tt IndPossibleDBPosR}$ 

Numeric vector containing the possible positions around a databot dependent on

the radius.

AllFreePosR0 NumericMatrix, see AllallowedDBPosR0 in setPolarGrid.

NumAllDB Integer total number of databots

Lines Integer stating the number of Lines the polar grid consists of.

Columns Integer stating the number of columns the polar grid consists of.

Origin Numeric origin of the positions of grid in two dimensions

Happiness Numeric value indicating the global happiness over all databots

GridRadii Numeric matrix with radius information of polar transformation for each grid

position

GridAngle Numeric matrix with angle information of polar transformation for each grid

position

QuadOrHexa optional, bool: If TRUE prints status every 100 iterations

RadiusVector Numeric vector stating all moving radius in a descending order (cooling down

scheme).

Rmin Integer stating minimum radius.

Rmax Integer stating maximum radius.

Cls Integer vector stating the classification vector for each datapoints/databots.

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Debug optional, bool: If TRUE prints information for debugging.

pp Numeric vector stating ratio of number of jumping simultaneously DataBots

of one eppoch (per nash-equilibirum), this vector is linearly monotonically de-

creasing.

PlotIt optional, bool: If TRUE creates plot of projection after each epoch.

Verbose optional, integer stating degree of textual feedback. 0 = no output, 1 = basic

notifications, 2 = progress bar, 3 = details.

#### **Details**

Algorithm is described in [Thrun, 2018, p. 95, Listing 8.1].

#### Value

list of

AllDataBotsPosRe

Numeric vector [1:n] of the current positions for the databots on first of two dimensions.

AllDataBotsPosIm

Numeric vector [1:n] of the current positions for the databots on second of two

dimensions.

CourseOfHappiness

Numeric Vector, states the global happiness value per epoch.

RadiusPerEpoch NumericVector, stating the radius used per epoch in order of computation.

## Author(s)

Quirin Stier

#### 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.

PswarmRadiusParallel Intern function, do not use yourself

#### **Description**

Finds the weak Nash equilibrium of the data bots for one epoch depending on a radius, which requires the setting of constants, grid, and so on in, see Pswarm.

#### Usage

PswarmRadiusParallel(DataBotsPos, DataDists, AllallowedDBPosR0, IndPossibleDBPosRe, IndPossibleDBPosIm, Lines, Columns, Radius, NumAllDB, NumChoDB, NumFreeShape1, NumJumps, Origin1, Origin2, Happiness, MinIterations, HappinessInclination, Eps, debug)

PswarmRadiusParallel 27

#### **Arguments**

DataBotsPos Numeric vector [1:NumJumps\*n\*2] containing the current positions and all po-

> sitions for considered/possible jumps which can be computed (depending on number of jumps parameter NumJumps) for the databots on two dimensions.

DataDists Numeric vector with vectorized distance matrix of the datapoints in the original

(high-dimensional) data space

AllallowedDBPosR0

NumericMatrix, see AllallowedDBPosR0 in setPolarGrid

IndPossibleDBPosRe

Numeric Vector of possible positions of the 1st coordinate.

IndPossibleDBPosIm

Numeric Vector of possible positions of the 2nd coordinate.

Lines Integer stating the number of Lines the polar grid consists of. Columns Integer stating the number of columns the polar grid consists of. Radius Numeric (Integer) stating the moving radius of the databots

NumAllDB Integer total number of databots

NumChoDB Integer number of databots chosen for moving/jumps.

NumFreeShape1 Integer stating the first dimension of the numeric matrix book keeping the pos-

sible position grid

NumJumps Integer number of jumps Origin1 Numeric origin coordinate 1 Origin2 Numeric origin coordinate 2

Happiness Numeric value indicating the global happiness over all databots

MinIterations asdf HappinessInclination

asdf

Eps optional, double: Stop criterion for convergence of each epoche.

debug optional, bool: If TRUE prints status every 100 iterations

## **Details**

Algorithm is described in [Thrun, 2018, p. 95, Listing 8.1].

#### Value

list of

AllDataBotsPos ComplexVector, indizes of DataBot Positions after a weak Nash equlibrium is

stressverlauf Numeric Vector, intern result, for debugging only

fokussiertlaufind

Numeric Vector, intern result, for debugging only

#### Author(s)

**Ouirin Stier** 

#### 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/Ultsch, 2021] Thrun, M. C., and Ultsch, A.: Swarm Intelligence for Self-Organized Clustering, Artificial Intelligence, Vol. 290, pp. 103237, doi:10.1016/j.artint.2020.103237, 2021.

[Stier/Thrun, 2024] Stier, Q. and Thrun, M. C.: An efficient multicore CPU implementation of the DatabionicSwarm, 18th conference of the International Federation of Classification Societies (IFCS), San José, Costa Rica, July 14-19, 2024.

PswarmRadiusSequential

intern function, do not use yourself

## Description

Finds the weak Nash equilibirium for DataBots in one epoch(Radius), requires the setting of constants, grid, and so on in Pswarm

## Usage

PswarmRadiusSequential(AllDataBotsPosOld, Radius, DataDists, IndPossibleDBPosR, RadiusPositionsschablone, pp, Nullpunkt, Lines, Columns, nBots, limit, steigungsverlaufind, Happiness, debug)

## **Arguments**

AllDataBotsPosOld

Complex Vector [1:n,1], DataBots position in the last Nash-Equlibriuum

Radius double, Radius of payoff function, neighborhood, where other DatsBots can be

smelled

DataDists NumericMatrix, Inputdistances[1:n,1:n]

IndPossibleDBPosR

Complex Vector, see output of findPossiblePositionsCsingle

RadiusPositionsschablone

NumericMatrix, see AllallowedDBPosR0 in setPolarGrid

pp NumericVector, number of jumping simultaneously DataBots of one eppoch

(per nash-equilibirum), this vector is linearly monotonically decreasing

Nullpunkt NumericVector, equals which(AllallowedDBPosR0==0,arr.ind=T), see see

AllallowedDBPosR0 in setPolarGrid

Lines double, small edge length of rectangulare grid
Columns double, big edge length of rectangulare grid

nBots double, intern constant, equals round(pp[Radius]\*DBAnzahl)

limit int, intern constant, equals ceiling(1/pp[Radius])

steigungsverlaufind

int, intern constant

Happiness double, intern constant, sum of payoff of all databots in random condition before

the algorithm starts

debug optional, bool: If TRUE prints status every 100 iterations

#### **Details**

Algorithm is described in [Thrun, 2018, p. 95, Listing 8.1].

#### Value

list of

AllDataBotsPos ComplexVector, indizes of DataBot Positions after a weak Nash equlibrium is

found

stressverlauf Numeric Vector, intern result, for debugging only

fokussiertlaufind

Numeric Vector, intern result, for debugging only

## 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.

rDistanceToroidCsingle

Intern function for Pswarm

## Description

toroid distance calculation

#### Usage

```
rDistanceToroidCsingle( AllDataBotsPosX, AllDataBotsPosY, AllallowedDBPosR0, Lines, Columns, Nullpunkt)
```

#### **Arguments**

AllDataBotsPosX

NumericVector [1:n,1], positions of on grid

AllDataBotsPosY

NumericVector [1:n,1], positions of on grid

AllallowedDBPosR0

NumericMatrix

Lines double
Columns double

Nullpunkt NumericVector

#### **Details**

Part of the algorithm described in [Thrun, 2018, p. 95, Listing 8.1].

#### Value

numeric matrix of toroid Distances[1:n,1:n]

## Note

do not use yourself

## 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.

#### See Also

Pswarm

RelativeDifference 31

RelativeDifference

Relative Difference

## **Description**

Calculates the difference between positive x and y values

## Usage

```
RelativeDifference(X, Y, epsilon = 10^-10,na.rm=FALSE)
```

## **Arguments**

X either a value or numerical vector of [1:n]
Y either a value or numerical vector of [1:n]
epsilon Optional, If both x and y are approximatly zero the output is also zero
Optional, function does not work with non finite values. If these cases should be automatically removed, set parameter TRUE

#### **Details**

Contrary to other approaches in this cases the range of values lies between [-2,2]. The approach is only valid for positive values of X and Y. The realtive difference R is defined with

$$R = \frac{Y - X}{0.5*(X+Y)}$$

Negative value indicate that X is higher than Y and positive values that X is lower than Y.

#### Value

R

#### Note

It can be combined with the GabrielClassificationError if a clear baseline is defined.

#### Author(s)

Michael Thrun

## References

Ultsch, A.: Is Log Ratio a Good Value for Measuring Return in Stock Investments? GfKl 2008, pp, 505-511, 2008.

32 RobustNormalization

#### See Also

GabrielClassificationError

#### **Examples**

```
x=c(1:5)
y=runif(5,min=1,max=10)
RelativeDifference(x,y)
```

RobustNormalization

RobustNormalization

#### **Description**

RobustNormalization as described in [Milligan/Cooper, 1988].

#### Usage

```
RobustNormalization(Data, Centered=FALSE, Capped=FALSE,
na.rm=TRUE, WithBackTransformation=FALSE,
pmin=0.01, pmax=0.99)
```

## **Arguments**

Data [1:n,1:d] data matrix of n cases and d features
Centered centered data around zero by median if TRUE

Capped TRUE: outliers are capped above 1 or below -1 and set to 1 or -1.

na.rm If TRUE, infinite vlaues are disregarded

WithBackTransformation

If in the case for forecasting with neural networks a backtransformation is re-

quired, this parameter can be set to 'TRUE'.

pmin defines outliers on the lower end of scale
pmax defines outliers on the higher end of scale

#### **Details**

Normalizes features either between -1 to 1 (Centered=TRUE) or 0-1 (Centered=TRUE) without changing the distribution of a feature itself. For a more precise description please read [Thrun, 2018, p.17].

"[The] scaling of the inputs determines the effective scaling of the weights in the last layer of a MLP with BP neural netowrk, it can have a large effect on the quality of the final solution. At the outset it is besto to standardize all inputs to have mean zero and standard deviation 1 [(or at least the range under 1)]. This ensures all inputs are treated equally in the regularization prozess, and allows to choose a meaningful range for the random starting weights."[Friedman et al., 2012]

RobustNormalization 33

#### Value

if WithBackTransformation=FALSE: TransformedData[1:n,1:d] i.e., normalized data matrix of n cases and d features

if WithBackTransformation=TRUE: List with

#### TransformedData

[1:n,1:d] normalized data matrix of n cases and d features

MinX [1:d] numerical vector used for manual back-transformation of each feature

MaxX [1:d] numerical vector used for manual back-transformation of each feature

Denom [1:d] numerical vector used for manual back-transformation of each feature

Center [1:d] numerical vector used for manual back-transformation of each feature

#### Author(s)

Michael Thrun

#### References

[Milligan/Cooper, 1988] Milligan, G. W., & Cooper, M. C.: A study of standardization of variables in cluster analysis, Journal of Classification, Vol. 5(2), pp. 181-204. 1988.

[Friedman et al., 2012] Friedman, J., Hastie, T., & Tibshirani, R.: The Elements of Statistical Learning, (Second ed. Vol. 1), Springer series in statistics New York, NY, USA:, ISBN, 2012.

[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.

#### See Also

RobustNorm BackTrafo

## **Examples**

```
Scaled = RobustNormalization(rnorm(1000, 2, 100), Capped = TRUE)
hist(Scaled)

m = cbind(c(1, 2, 3), c(2, 6, 4))
List = RobustNormalization(m, FALSE, FALSE, FALSE, TRUE)
TransformedData = List$TransformedData

mback = RobustNorm_BackTrafo(TransformedData, List$MinX, List$Denom, List$Center)
sum(m - mback)
```

## Description

Transforms the Robust Normalization back if Capped=FALSE

## Usage

```
RobustNorm_BackTrafo(TransformedData,
MinX,Denom,Center=0)
```

## **Arguments**

TransformedData

[1:n,1:d] matrix

MinX scalar
Denom scalar
Center scalar

#### **Details**

For details see RobustNormalization

#### Value

```
[1:n,1:d] Data matrix
```

#### Author(s)

Michael Thrun

#### See Also

RobustNormalization

## **Examples**

sESOM4BMUs 35

sESOM4BMUs Intern function: Simplified Emergent Self-Organizing Ma	p
--	---

#### **Description**

Intern function for the simplified ESOM (sESOM) algorithm for fixed BestMatchingUnits.

## Usage

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

## Arguments

BMUs [1:Lines,1:Columns], BestMAtchingUnits 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 ListAsEsomNeu-

rons()

toroid TRUE/FALSE - topology of points

CurrentRadius number between 1 to x

ComputeInR =T: Rcode, =F Cpp Code.

Parallel Optional, =TRUE: Parallel C++ implementation, =FALSE C++ implementation

#### **Details**

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

## Value

esom numeric 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, doi:10.1007/9783658205409, 2018.

36 setGridSize

#### See Also

#### GeneratePswarmVisualization

setdiffMatrix shortens Matrix2Curt by those rows that are in both ma-

trices.

#### **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)

CL,MT 12/2014

setGridSize Sets the grid size for the Pswarm algorithm

## Description

Automatically sets the size of the grid, formula see [Thrun, 2018, p. 93-94].

## Usage

```
setGridSize(InputDistances,minp=0.01,maxp=0.99,alpha=4, Verbose = 0)
```

## Arguments

 ${\tt InputDistances} \quad \hbox{$[1:n,1:n]$ symmetric matrix of input distances}$ 

minp default value: 0.01, see quantile, first value in the vector of probs estimates

robust minimum of distances

maxp default value: 0.99, see quantile, last value of the vector of probs estimates

robust maximum of distances

alpha Do not change! Intern parameter, Only if Java Version of Pswarm instead of

C++ version is used.

Verbose optional, integer stating degree of textual feedback. 0 = no output, 1 = basic

notifications, 2 = progress bar, 3 = details.

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#### **Details**

grid is set such that minimum and maximum distances can be shown on the grid

#### Value

LC=c(Lines, Columns) size of the grid for Pswarm

#### Author(s)

Michael Thrun, Florian Lerch

#### 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.

#### See Also

automatic choice of LC for Pswarm

#### **Examples**

```
data("Lsun3D")
Data=Lsun3D$Data
Cls=Lsun3D$Cls
InputDistances=as.matrix(dist(Data))
#If not called separately setGridSize() is called in Pswarm
LC=setGridSize(InputDistances)
```

setPolarGrid

*Intern function: Sets the polar grid* 

## **Description**

Sets a polar grid for a swarm in an rectangular shape

## Usage

setPolarGrid(Lines,Columns,QuadOrHexa,PlotIt,global)

#### **Arguments**

Lines Integer, hast to be able to be divided by 2

Columns Integer, with Columns>=Lines

QuadOrHexa bool, default(TRUE) If False Hexagonal grid, default quad grid

PlotIt bool, default(FALSE)

global bool, default(TRUE), intern parameter, how shall the radii be calculated?

38 setRmin

#### **Details**

Part of the Algorithm described in [Thrun, 2018, p. 95, Listing 8.1].

#### Value

list of

GridRadii matrix [1:Lines,1:Columns], Radii Matrix of all possible Positions of DataBots

in Grid

GridAngle matrix [1:Lines,1:Columns], Angle Matrix of all possible Positions of DataBots

in Grid

AllallowedDBPosR0

matrix [1:Lines+1,1:Columns+1], Matrix of radii in polar coordinates respecting

origin (0,0) of all allowed DataBots Positions in one jump

AllallowedDBPosPhi0

matrix [1:Lines+1,1:Columns+1], # V\$AllallowedDBPosPhi0[Lines+1,Lines+1] Matrix of angle in polar coordinates respecting origin (0,0) of all allowed DataBots

Positions in one jump

#### 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.

## See Also

Pswarm

setRmin

Intern function: Estimates the minimal radius for the Databot scent

## **Description**

estimates the minimal radius on apolar grid in the automated annealing process of Pswarm, details of how can be read in [Thrun, 2018, p. 97]

ShortestGraphPathsC 39

#### **Arguments**

Lines x-value determining the size of the map, i.e. how many open places for DataBots

will be available on the 2-dimensional grid BEWARE: has to be able to be di-

vided by 2

Columns y-value determining the size of the map, i.e. how many open places for DataBots

will be available on the 2-dimensional grid Columns>Lines

AllallowedDBPosR0

[1:Lines+1,1:Lines+1]Matrix of radii in polar coordinates respecting origin (0,0)

of all allowed DataBots Positions in one jump

p percent of gitterpositions, which should be considered

#### Value

Rmin Minimum Radius

#### 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.

ShortestGraphPathsC

 $Shortest\ GraphPaths = geodesic\ distances$ 

## **Description**

Dijkstra's SSSP (Single source shortest path) algorithm, from all points to all points

## Usage

ShortestGraphPathsC(Adj, Cost)

#### **Arguments**

Adj [1:n,1:n] 0/1 adjascency matrix, e.g. from delaunay graph or gabriel graph

Cost [1:n,1:n] matrix, distances between n points (normally euclidean)

#### **Details**

Vertices are the points, edges have the costs defined by weights (normally a distance). The algorithm runs in runs in O(n\*E\*Log(V)), see also [Jungnickel, 2013, p. 87]. Further details can be found in [Jungnickel, 2013, p. 83-87] and [Thrun, 2018, p. 12].

40 trainstepC

#### Value

ShortestPaths[1:n,1:n] vector, shortest paths (geodesic) to all other vertices including the source vertice itself from al vertices to all vertices, stored as a matrix

#### Note

require C++11 standard (set flag in Compiler, if not set automatically)

#### Author(s)

Michael Thrun

#### References

[Dijkstra,1959] Dijkstra, E. W.: A note on two problems in connexion with graphs, Numerische mathematik, Vol. 1(1), pp. 269-271. 1959.

[Jungnickel, 2013] Jungnickel, D.: Graphs, networks and algorithms, (4th ed ed. Vol. 5), Berlin, Heidelberg, Germany, Springer, ISBN: 978-3-642-32278-5, 2013.

[Thrun/Ultsch, 2017] Thrun, M.C., Ultsch, A.: Projection based Clustering, Conf. Int. Federation of Classification Societies (IFCS),DOI:10.13140/RG.2.2.13124.53124, Tokyo, 2017.

[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.

## See Also

DijkstraSSSP

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, NoCases)

## Arguments

VX	array [1:Lines,1:Columns,1:Weights], WeightVectors that will be trained, inter-
	nally 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

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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?

NoCases int, number of samples in the given non-sampled dataset

#### **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, 2018.

trainstepC2	internal function for s-esom	

## **Description**

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

## Usage

trainstepC2(esomwts,aux, DataSampled,BMUsampled,Lines,Columns, Weights, Radius, toroid, NoCases) 42 trainstepC2

## **Arguments**

esomwts array [1:Lines,1:Columns,1:Weights], WeightVectors that will be trained, inter-

nally transformed von NumericVector to cube

aux 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
Weights double, number of weights

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?

NoCases int, number of samples in the given non-sampled dataset

#### **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, 2018.

UniquePoints 43

UniquePoints	Unique Points	

#### **Description**

return only the unique points in Datapoints

## Usage

```
UniquePoints(Datapoints, Eps=1e-10)
```

## **Arguments**

Datapoints [1:n,1:d] matrix of Datapoints points of dimension d, the points are in the rows

Eps Optional, scalar above zero that defines minimum non-identical euclidean dis-

tance between two points

#### **Details**

Euclidean distance is computed and used within. Setting Eps to a very small number results in the identification of unique data points. Setting epsilon to a higher number results in the definition of mesh points within an d-dimensional R-ball graph.

#### Value

List with

Unique [1:k,1:d] Datapoints points without duplicate points

IsDuplicate [1:n,1:n] matrix,for i!=j IsDuplicate[i,j]== 1 if Datapoints[i,] == Datapoints[j,]

IsDuplicate[i,i]==0

UniqueInd [1:k] index vector such that Unique == Datapoints[UniqueInd,], it has k non-

consecutive numbers or labels, each label defines a row number within Data-

points[1:n,1:d] of a unique data point

Uniq2DatapointsInd

[1:n] index vector. It has k unique index numbers representing the arbitrary labels. Each labels is mapped uniquely to a point in Unique. Logically in a way such that Datapoints == Unique[Uniq2DatapointsInd,] (will not work directly

in R this way)

#### Author(s)

Michael Thrun

## **Examples**

```
Datapoints2D=rbind(c(1,2),c(1,2),c(1,3),c(3,1))
V=UniquePoints(Datapoints2D)
```

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