Package ‘dimRed’

October 13, 2022

Title  A Framework for Dimensionality Reduction
Version  0.2.6
Description  A collection of dimensionality reduction
              techniques from R packages and a common
              interface for calling the methods.
Depends  R (>= 3.0.0), DRR
Imports  magrittr, methods
Suggests  NMF, MASS, Matrix, RANN, RSpectra, Rtsne, cccd, coRanking,
          diffusionMap, energy, fastICA, ggplot2, graphics, igrap,
          keras, kernlab, knitr, loe, optimx, pcaL1, pcaPP, reticulate,
          rgl, scales, scatterplot3d, stats, tensorflow, testthat, tidyR,
          tinytex, umap, vegan
VignetteBuilder  knitr
License  GPL-3 | file LICENSE
BugReports  https://github.com/gdkrmr/dimRed/issues
URL  https://www.guido-kraemer.com/software/dimred/
Encoding  UTF-8
Collate  'dimRedMethod-class.R' 'misc.R' 'dimRedData-class.R'
         'dimRedResult-class.R' 'autoencoder.R' 'dataSets.R' 'diffmap.R'
         'dimRed.R' 'drr.R' 'embed.R' 'fastica.R' 'get_info.R'
         'graph_embed.R' 'hle.R' 'isomap.R' 'kpca.R' 'l1pca.R' 'leim.R'
         'lle.R' 'loe.R' 'mds.R' 'mixColorSpaces.R' 'nmds.R' 'nmf.R'
         'pca.R' 'plot.R' 'quality.R' 'rotate.R' 'soe.R' 'tsne.R'
         'umap.R'
RoxygenNote  7.2.0
Config/testthat/edition  3
NeedsCompilation  yes
Author  Guido Kraemer [aut, cre]
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Repository  CRAN
Date/Publication  2022-07-11 12:40:06 UTC
R topics documented:

- dimRed-package .................................................. 3
- as.data.frame ..................................................... 4
- as.dimRedData .................................................... 4
- AUC_LnK_R_NX,dimRedResult-method .................. 5
- AutoEncoder-class .............................................. 6
- cophenetic_correlation,dimRedResult-method .......... 8
- dataSets ........................................................... 9
- DiffusionMaps-class .......................................... 10
- dimRedData-class ............................................... 11
- dimRedMethod-class .......................................... 13
- dimRedMethodList ............................................ 14
- dimRedResult-class ........................................... 15
- distance_correlation,dimRedResult-method ........... 17
- DrL-class .......................................................... 18
- DRR-class ........................................................ 19
- embed ............................................................... 21
- FastICA-class ................................................... 23
- FruchtermanReingold-class .................................. 24
- getData ............................................................. 26
- getDimRedData .................................................. 26
- getMeta ............................................................. 26
- getNDim ............................................................. 27
- getOrgData ........................................................ 27
- getOtherData ..................................................... 27
- getPars ............................................................. 28
- getRotationMatrix ............................................. 28
- HLLE-class ........................................................ 29
- installSuggests .................................................. 30
- Isomap-class ....................................................... 31
- KamadaKawai-class ............................................ 32
- kPCA-class ........................................................ 34
- LaplacianEigenmaps-class ................................... 35
- LCMC,dimRedResult-method ................................. 36
- makeKNNgraph .................................................... 37
- maximize_correlation,dimRedResult-method ............ 38
- MDS-class .......................................................... 38
- mean_R_NX,dimRedResult-method ............................ 40
- mixColorRamps ................................................... 40
- ndims ................................................................. 41
- nMDS-class ........................................................ 42
- NNMF-class ........................................................ 43
- PCA-class ........................................................... 44
- PCA_L1-class ....................................................... 46
- plot ................................................................. 47
- plot_R_NX .......................................................... 48
- print ................................................................. 50
The dimRed package

Description

This package simplifies dimensionality reduction in R by providing a framework of S4 classes and methods. dimRed collects dimensionality reduction methods that are implemented in R and implements others. It gives them a common interface and provides plotting functions for visualization and functions for quality assessment.

Funding provided by the Department for Biogeochemical Integration, Empirical Inference of the Earth System Group, at the Max Plack Institute for Biogeochemistry, Jena.

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References


See Also

Useful links:

- https://www.guido-kraemer.com/software/dimred/
- Report bugs at https://github.com/gdkrmr/dimRed/issues
as.data.frame

Converts to data.frame

Description

General conversions of objects created by dimRed to data.frame. See class documentations for details (dimRedData, dimRedResult). For the documentation of this function in base package, see here: as.data.frame.default.

Usage

as.data.frame(x, row.names, optional, ...)

Arguments

x The object to be converted
row.names unused in dimRed
optional unused in dimRed
... other arguments.

as.dimRedData

Converts to dimRedData

Description

Conversion functions to dimRedData.

Usage

as.dimRedData(formula, ...)

## S4 method for signature 'formula'
as.dimRedData(formula, data)

Arguments

formula The formula, left hand side is assigned to the meta slot right hand side is assigned to the data slot.
... other arguments.
data Will be coerced into a data.frame with as.data.frame

Methods (by class)

- formula: Convert a data.frame to a dimRedData object using a formula
See Also

Other dimRedData: dimRedData-class

Examples

```r
## create a dimRedData object using a formula
as.dimRedData(Species ~ Sepal.Length + Sepal.Width + Petal.Length + Petal.Width,
              iris)[1:5]
```

Description

Calculate the Area under the R_NX(ln K), used in Lee et. al. (2015). Note that despite the name, this does not weight the mean by the logarithm, but by 1/K. If explicit weighting by the logarithm is desired use weight = “log” or weight = “log10”

Usage

```r
## S4 method for signature 'dimRedResult'
AUC_inK_R_NX(object, weight = "inv")
```

Arguments

- `object` of class dimRedResult
- `weight` the weight function used, one of c("inv", "log", "log10")

Details

The naming confusion originated from equation 17 in Lee et al (2015) and the name of this method may change in the future to avoid confusion.

References


See Also

AutoEncoder-class

Description

An S4 Class implementing an Autoencoder

Details

Autoencoders are neural networks that try to reproduce their input. Consider this method unstable, as the internals may still be changed.

Slots

fun A function that does the embedding and returns a dimRedResult object.
stdpars The standard parameters for the function.

General usage

Dimensionality reduction methods are S4 Classes that either be used directly, in which case they have to be initialized and a full list with parameters has to be handed to the @fun() slot, or the method name be passed to the embed function and parameters can be given to the . . . , in which case missing parameters will be replaced by the ones in the @stdpars.

Parameters

Autoencoder can take the following parameters:

ndim The number of dimensions for reduction.
n_hidden The number of neurons in the hidden layers, the length specifies the number of layers, the length must be impair, the middle number must be the same as ndim.
activation The activation functions for the layers, one of "tanh", "sigmoid", "relu", "elu", everything else will silently be ignored and there will be no activation function for the layer.
weight_decay the coefficient for weight decay, set to 0 if no weight decay desired.
learning_rate The learning rate for gradient descend
graph Optional: A list of bits and pieces that define the autoencoder in tensorflow, see details.
keras_graph Optional: A list of keras layers that define the encoder and decoder, specifying this, will ignore all other topology related variables, see details.
batchsize If NA, all data will be used for training, else only a random subset of size batchsize will be used
n_steps the number of training steps.
Details

There are several ways to specify an autoencoder, the simplest is to pass the number of neurons per layer in `n_hidden`, this must be a vector of integers of impair length and it must be symmetric and the middle number must be equal to `ndim`. For every layer an activation function can be specified with `activation`. For regularization weight decay can be specified by setting `weight_decay > 0`. Currently only a gradient descent optimizer is used, the learning rate can be specified by setting `learning_rate`. The learner can operate on batches if `batchsize` is not `NA`. The number of steps the learner uses is specified using `n_steps`.

Further training a model

If the model did not converge in the first training phase or training with different data is desired, the `dimRedResult` object may be passed as `autoencoder` parameter; In this case all topology related parameters will be ignored.

Using Keras layers

The encoder and decoder part can be specified using a list of `keras` layers. This requires a list with two entries, `encoder` should contain a LIST of keras layers WITHOUT the `layer_input` that will be concatenated in order to form the encoder part. `decoder` should be defined accordingly, the output of `decoder` must have the same number of dimensions as the input data.

Using Tensorflow

The model can be entirely defined in `tensorflow`, it must contain a list with the following entries:

- `encoder` A tensor that defines the encoder.
- `decoder` A tensor that defines the decoder.
- `network` A tensor that defines the reconstruction (encoder + decoder).
- `loss` A tensor that calculates the loss (network + loss function).
- `in_data` A placeholder that points to the data input of the network AND the encoder.
- `in_decoder` A placeholder that points to the input of the decoder.
- `session` A `tensorflow` Session object that holds the values of the tensors.

Implementation

Uses `tensorflow` as a backend, for details an problems relating tensorflow, see [https://tensorflow.rstudio.com](https://tensorflow.rstudio.com).

See Also

Other dimensionality reduction methods: DRR-class, DiffusionMaps-class, DrL-class, FastICA-class, FruchtermanReingold-class, HLLE-class, Isomap-class, KamadaKawai-class, MDS-class, NNMF-class, PCA-class, PCA_L1-class, UMAP-class, dimRedMethod-class, dimRedMethodList(), kPCA-class, nMDS-class, tSNE-class
Examples

```r
## Not run:
dat <- loadDataSet("3D S Curve")
emb <- embed(dat, "AutoEncoder")

# predicting is possible:
samp <- sample(floor(nrow(dat) / 10))
emb2 <- embed(dat[samp])
emb3 <- predict(emb2, dat[-samp])

plot(emb, type = "2vars")
plot(emb2, type = "2vars")
points(getData(emb3))

## End(Not run)
```

cophenetic_correlation, dimRedResult-method

Method cophenetic_correlation

Description

Calculate the correlation between the distance matrices in high and low dimensional space.

Usage

```r
## S4 method for signature 'dimRedResult'
cophenetic_correlation(object, d = stats::dist, cor_method = "pearson")
```

Arguments

- `object`: of class dimRedResult
- `d`: the distance function to use.
- `cor_method`: The correlation method.

See Also

Example Data Sets for dimensionality reduction

Description
A compilation of standard data sets that are often being used to showcase dimensionality reduction techniques.

Usage
loadDataSet(name = dataSetList(), n = 2000, sigma = 0.05)

dataSetList()

Arguments
name
A character vector that specifies the name of the data set.
n
In generated data sets the number of points to be generated, else ignored.
sigma
In generated data sets the standard deviation of the noise added, else ignored.

Details
The argument name should be one of dataSetList(). Partial matching is possible, see match.arg. Generated data sets contain the internal coordinates of the manifold in the meta slot. Call dataSetList() to see what data sets are available.

Value
loadDataSet an object of class dimRedData. dataSetList() return a character string with the implemented data sets

Examples
## a list of available data sets:
dataSetList()

## Load a data set:
swissRoll <- loadDataSet("Swiss Roll")

if(requireNamespace("scatterplot3d", quietly = TRUE))
  plot(swissRoll, type = "3vars")

## Load Iris data set, partial matching:
loadDataSet("I")
DiffusionMaps-class  Diffusion Maps

Description

An S4 Class implementing Diffusion Maps

Details

Diffusion Maps uses a diffusion probability matrix to robustly approximate a manifold.

Slots

fun  A function that does the embedding and returns a dimRedResult object.
stdpars  The standard parameters for the function.

General usage

Dimensionality reduction methods are S4 Classes that either be used directly, in which case they have to be initialized and a full list with parameters has to be handed to the @fun() slot, or the method name be passed to the embed function and parameters can be given to the ..., in which case missing parameters will be replaced by the ones in the @stdpars.

Parameters

Diffusion Maps can take the following parameters:

- **d**  a function transforming a matrix row wise into a distance matrix or dist object, e.g. dist.
- **ndim**  The number of dimensions
- **eps**  The epsilon parameter that determines the diffusion weight matrix from a distance matrix d, \( \exp(-d^2/\text{eps}) \), if set to "auto" it will be set to the median distance to the 0.01*n nearest neighbor.
- **t**  Time-scale parameter. The recommended value, 0, uses multiscale geometry.
- **delta**  Sparsity cut-off for the symmetric graph Laplacian, a higher value results in more sparsity and faster calculation. The predefined value is \( 10^{-5} \).

Implementation

Wraps around diffuse, see there for details. It uses the notation of Richards et al. (2009) which is slightly different from the one in the original paper (Coifman and Lafon, 2006) and there is no \( \alpha \) parameter. There is also an out-of-sample extension, see examples.

References


See Also

Other dimensionality reduction methods: AutoEncoder-class, DRR-class, DrL-class, FastICA-class, FruchtermanReingold-class, HLLE-class, Isomap-class, KamadaKawai-class, MDS-class, NNMF-class, PCA-class, PCA_L1-class, UMAP-class, dimRedMethod-class, dimRedMethodList(), kPCA-class, nMDS-class, tSNE-class

Examples

```r
if(requireNamespace("diffusionMap", quietly = TRUE)) {
  dat <- loadDataSet("3D S Curve", n = 300)
  emb <- embed(dat, "DiffusionMaps")

  plot(emb, type = "2vars")

  # predicting is possible:
  samp <- sample(floor(nrow(dat) / 10))
  emb2 <- embed(dat[samp])
  emb3 <- predict(emb2, dat[-samp])

  plot(emb2, type = "2vars")
  points(getData(emb3))
}
```

Description

A class to hold data for dimensionality reduction and methods.

Usage

```r
## S4 method for signature 'dimRedData'
as.data.frame(x, meta.prefix = "meta.", data.prefix = "")

## S4 method for signature 'dimRedData'
getData(object)

## S4 method for signature 'dimRedData'
getMeta(object)

## S4 method for signature 'dimRedData'
nrow(x)

## S4 method for signature 'dimRedData,ANY,ANY,ANY'
x[i]

## S4 method for signature 'dimRedData'
n dims(object)
```
Arguments

- **x**: Of class `dimRedData`
- **meta.prefix**: Prefix for the columns of the meta data names.
- **data.prefix**: Prefix for the columns of the variable names.
- **object**: Of class `dimRedData`.
- **i**: A valid index for subsetting rows.

Details

The class has two slots, `data` and `meta`. The `data` slot contains a numeric matrix with variables in columns and observations in rows. The `meta` slot may contain a `data.frame` with additional information. Both slots need to have the same number of rows or the `meta` slot needs to contain an empty `data.frame`.

See examples for easy conversion from and to `data.frame`.

For plotting functions see `plot.dimRedData`.

Methods (by generic)

- `as.data.frame`: convert to `data.frame`
- `getData`: Get the data slot.
- `getMeta`: Get the meta slot.
- `nrow`: Get the number of observations.
- `[`: Subset rows.
- `ndims`: Extract the number of Variables from the data.

Slots

- **data**: of class `matrix`, holds the data, observations in rows, variables in columns
- **meta**: of class `data.frame`, holds meta data such as classes, internal manifold coordinates, or simply additional data of the data set. Must have the same number of rows as the `data` slot or be an empty `data.frame`.

See Also

Other `dimRedData`: `as.dimRedData()`

Examples

```r
## Load an example data set:
s3d <- loadDataSet("3D S Curve")

## Create using a constructor:
### without meta information:
dimRedData(iris[, 1:4])
```
### with meta information:
dimRedData(iris[, 1:4], iris[, 5])

### using slot names:
dimRedData(data = iris[, 1:4], meta = iris[, 5])

## Convert to a dimRedData objects:
Iris <- as(iris[, 1:4], "dimRedData")

## Convert to data.frame:
head(as(s3d, "data.frame"))
head(as.data.frame(s3d))
head(as.data.frame(as(iris[, 1:4], "dimRedData")))

## Extract slots:
head(getData(s3d))
head(getMeta(s3d))

## Get the number of observations:
nrow(s3d)

## Subset:
s3d[1:5, ]

## Shuffle data:
s3 <- s3d[nrow(s3d)]

## Get the number of variables:
ndims(s3d)

---

**dimRedMethod-class**  Class "dimRedMethod"

**Description**

A virtual class "dimRedMethod" to serve as a template to implement methods for dimensionality reduction.

**Details**

Implementations of dimensionality reductions should inherit from this class.

The **fun** slot should be a function that takes three arguments

- **data** An object of class dimRedData.
- **pars** A list with the standard parameters.
- **keep.org.data** Logical. If the original data should be kept in the output.
and returns an object of class `dimRedResult`.
The `stdpars` slot should take a list that contains standard parameters for the implemented methods. This way the method can be called by `embed(data, "method-name",...)`, where `...` can be used to change single parameters.

**Slots**

- **fun** A function that does the embedding.
- **stdpars** A list with the default parameters for the `fun` slot.
- **requires** A vector with all packages R packages that need to be installed to run the method. In some occasions a method may work without one of the packages. Does not include Python dependencies such as Tensorflow. Used to auto skip tests

**See Also**

Other dimensionality reduction methods: `AutoEncoder-class`, `DRR-class`, `DiffusionMaps-class`, `DrL-class`, `FastICA-class`, `FruchtermanReingold-class`, `HLLE-class`, `Isomap-class`, `KamadaKawai-class`, `MDS-class`, `NNMF-class`, `PCA-class`, `PCA_L1-class`, `UMAP-class`, `dimRedMethodList()`, `kPCA-class`, `nMDS-class`, `tSNE-class`

---

**Description**

Get the names of all methods for dimensionality reduction.

**Usage**

`dimRedMethodList(filter = FALSE)`

**Arguments**

- **filter** filter methods by methods that have their dependencies installed

**Details**

Returns the name of all classes that inherit from `dimRedMethod-class` to use with `embed`.

**Value**

a character vector with the names of classes that inherit from `dimRedMethod`.

**See Also**

Other dimensionality reduction methods: `AutoEncoder-class`, `DRR-class`, `DiffusionMaps-class`, `DrL-class`, `FastICA-class`, `FruchtermanReingold-class`, `HLLE-class`, `Isomap-class`, `KamadaKawai-class`, `MDS-class`, `NNMF-class`, `PCA-class`, `PCA_L1-class`, `UMAP-class`, `dimRedMethod-class`, `kPCA-class`, `nMDS-class`, `tSNE-class`
Examples

    dimRedMethodList()

---

dimRedResult-class  

Class "dimRedResult"

Description

A class to hold the results of a dimensionality reduction.

Usage

    ## S4 method for signature 'dimRedResult'
    predict(object, xnew)

    ## S4 method for signature 'dimRedResult'
    inverse(object, ynew)

    ## S4 method for signature 'dimRedResult'
    as.data.frame(
        x,
        org.data.prefix = "org.",
        meta.prefix = "meta.",
        data.prefix = ""
    )

    ## S4 method for signature 'dimRedResult'
    getPars(object)

    ## S4 method for signature 'dimRedResult'
    getNDim(object)

    ## S4 method for signature 'dimRedResult'
    print(x)

    ## S4 method for signature 'dimRedResult'
    getOrgData(object)

    ## S4 method for signature 'dimRedResult'
    getDimRedData(object)

    ## S4 method for signature 'dimRedResult'
    ndims(object)

    ## S4 method for signature 'dimRedResult'
    getOtherData(object)
Arguments

- **object**  Of class `dimRedResult`
- **xnew**  new data, of type `dimRedData`
- **ynew**  embedded data, of type `dimRedData`
- **x**  Of class `dimRedResult`
- **org.data.prefix**  Prefix for the columns of the `org.data` slot.
- **meta.prefix**  Prefix for the columns of `x@data@meta`.
- **data.prefix**  Prefix for the columns of `x@data@data`.

Methods (by generic)

- **predict**: apply a trained method to new data, does not work with all methods, will give an error if there is no `apply`. In some cases the apply function may only be an approximation.
- **inverse**: inverse transformation of embedded data, does not work with all methods, will give an error if there is no `inverse`. In some cases the apply function may only be an approximation.
- **as.data.frame**: convert to `data.frame`
- **getPars**: Get the parameters with which the method was called.
- **getNDim**: Get the number of embedding dimensions.
- **print**: Method for printing.
- **getOrgData**: Get the original data and meta.data
- **getDimRedData**: Get the embedded data
- **ndims**: Extract the number of embedding dimensions.
- **getOtherData**: Get other data produced by the method

Slots

- **data**  Output data of class `dimRedData`.
- **org.data**  original data, a matrix.
- **apply**  a function to apply the method to out-of-sample data, may not exist.
- **inverse**  a function to calculate the original coordinates from reduced space, may not exist.
- **has.org.data**  logical, if the original data is included in the object.
- **has.apply**  logical, if a forward method is exists.
- **has.inverse**  logical if an inverse method exists.
- **method**  saves the method used.
- **pars**  saves the parameters used.
- **other.data**  other data produced by the method, e.g. a distance matrix.
Examples

```r
## Create object by embedding data
iris.pca <- embed(loadDataSet("Iris"), "PCA")

## Convert the result to a data.frame
head(as(iris.pca, "data.frame"))
head(as.data.frame(iris.pca))

## There are no nameclashes to avoid here:
head(as.data.frame(iris.pca,
    org.data.prefix = "",
    meta.prefix = "",
    data.prefix = ""))

## Print it more or less nicely:
print(iris.pca)

## Get the embedded data as a dimRedData object:
getDimRedData(iris.pca)

## Get the original data including meta information:
getOrgData(iris.pca)

## Get the number of variables:
ndims(iris.pca)
```

---

distance_correlation,dimRedResult-method

**Method distance_correlation**

**Description**

Calculate the distance correlation between the distance matrices in high and low dimensional space.

**Usage**

```r
## S4 method for signature 'dimRedResult'
distance_correlation(object)
```

**Arguments**

- `object` of class `dimRedResult`

**See Also**

Description

An S4 Class implementing Distributed recursive Graph Layout.

Details

DrL uses a complex algorithm to avoid local minima in the graph embedding which uses several steps.

Slots

fun  A function that does the embedding and returns a dimRedResult object.
stdpars  The standard parameters for the function.

General usage

Dimensionality reduction methods are S4 Classes that either be used directly, in which case they have to be initialized and a full list with parameters has to be handed to the @fun() slot, or the method name be passed to the embed function and parameters can be given to the . . . , in which case missing parameters will be replaced by the ones in the @stdpars.

Parameters

DrL can take the following parameters:

ndim  The number of dimensions, defaults to 2. Can only be 2 or 3
knn  Reduce the graph to keep only the neares neighbors. Defaults to 100.
d  The distance function to determine the weights of the graph edges. Defaults to euclidean distances.

Implementation

Wraps around layout_with_drl. The parameters maxiter, epsilon and kkconst are set to the default values and cannot be set, this may change in a future release. The DimRed Package adds an extra sparsity parameter by constructing a knn graph which also may improve visualization quality.

References

**See Also**

Other dimensionality reduction methods: AutoEncoder-class, DRR-class, DiffusionMaps-class, FastICA-class, FruchtermanReingold-class, HLLE-class, Isomap-class, KamadaKawai-class, MDS-class, NMF-class, PCA-class, PCA_L1-class, UMAP-class, dimRedMethod-class, dimRedMethodList(), kPCA-class, nMDS-class, tSNE-class

**Examples**

```r
## Not run:
if(requireNamespace(c("igraph", "coRanking"), quietly = TRUE)) {

dat <- loadDataSet("Swiss Roll", n = 200)
emb <- embed(dat, "DrL")
plot(emb, type = "2vars")
}

## End(Not run)
```

---

**DRR-class**  
*Dimensionality Reduction via Regression*

**Description**

An S4 Class implementing Dimensionality Reduction via Regression (DRR).

**Details**

DRR is a non-linear extension of PCA that uses Kernel Ridge regression.

**Slots**

- `fun` A function that does the embedding and returns a dimRedResult object.
- `stdpars` The standard parameters for the function.

**General usage**

Dimensionality reduction methods are S4 Classes that either be used directly, in which case they have to be initialized and a full list with parameters has to be handed to the `@fun()` slot, or the method name be passed to the embed function and parameters can be given to the `. . .`, in which case missing parameters will be replaced by the ones in the `@stdpars`. 
Parameters

DRR can take the following parameters:

- **ndim**  The number of dimensions
- **lambda**  The regularization parameter for the ridge regression.
- **kernel**  The kernel to use for KRR, defaults to "rbfdot".
- **kernel.pars**  A list with kernel parameters, elements depend on the kernel used, "rbfdot" uses "sigma".
- **pca**  logical, should an initial pca step be performed, defaults to TRUE.
- **pca.center**  logical, should the data be centered before the pca step. Defaults to TRUE.
- **pca.scale**  logical, should the data be scaled before the pca step. Defaults to FALSE.
- **fastcv**  logical, should fastCV from the CVST package be used instead of normal cross-validation.
- **fastcv.test**  If fastcv = TRUE, separate test data set for fastcv.
- **cv.folds**  if fastcv = FALSE, specifies the number of folds for cross-validation.
- **fastkrr.nblocks**  integer, higher values sacrifice numerical accuracy for speed and less memory, see below for details.
- **verbose**  logical, should the cross-validation results be printed out.

Implementation

Wraps around drr, see there for details. DRR is a non-linear extension of principal components analysis using Kernel Ridge Regression (KRR, details see constructKRRLearner and constructFastKRRLearner). Non-linear regression is used to explain more variance than PCA. DRR provides an out-of-sample extension and a backward projection.

The most expensive computations are matrix inversions therefore the implementation profits a lot from a multithreaded BLAS library. The best parameters for each KRR are determined by cross-validaton over all parameter combinations of lambda and kernel.pars, using less parameter values will speed up computation time. Calculation of KRR can be accelerated by increasing fastkrr.nblocks, it should be smaller than n^1/3 up to sacrificing some accuracy, for details see constructFastKRRLearner. Another way to speed up is to use pars$fastcv = TRUE which might provide a more efficient way to search the parameter space but may also miss the global maximum, I have not ran tests on the accuracy of this method.

References


See Also

Other dimensionality reduction methods: AutoEncoder-class, DiffusionMaps-class, DrL-class, FastICA-class, FruchtermanReingold-class, HLLE-class, Isomap-class, KamadaKawai-class, MDS-class, NNMF-class, PCA-class, PCA_L1-class, UMAP-class, dimRedMethod-class, dimRedMethodList(), kPCA-class, nMDS-class, tSNE-class
Examples

```r
## Not run:
if(requireNamespace(c("kernlab", "DRR"), quietly = TRUE)) {

dat <- loadDataSet("variable Noise Helix", n = 200)[sample(200)]

emb <- embed(dat, "DRR", ndim = 3)

plot(dat, type = "3vars")
plot(emb, type = "3vars")

# We even have function to reconstruct, also working for only the first few dimensions
rec <- inverse(emb, getData(getDimRedData(emb))[, 1, drop = FALSE])
plot(rec, type = "3vars")
}

## End(Not run)
```

---

**embed**

*dispatches the different methods for dimensionality reduction*

**Description**

wraps around all dimensionality reduction functions.

**Usage**

```r
embed(.data, ...)
```

---

**S4 method for signature 'formula'**

```r
embed(
  .formula,
  .data,
  .method = dimRedMethodList(),
  .mute = character(0),
  .keep.org.data = TRUE,
  ...
)
```

**S4 method for signature 'ANY'**

```r
embed(
  .data,
  .method = dimRedMethodList(),
  .mute = character(0),
  .keep.org.data = TRUE,
  ...
)
## S4 method for signature 'dimRedData'

`embed(`
- `.data`,
- `.method = dimRedMethodList()`,
- `.mute = character(0)`,
- `.keep.org.data = TRUE`,
- `...`
`)

### Arguments

- `.data` object of class `dimRedData`, will be converted to be of class `dimRedData` if necessary; see examples for details.
- `...` the parameters, internally passed as a list to the dimensionality reduction method as `pars = list(...)`
- `.formula` a formula, see `as.dimRedData`.
- `.method` character vector naming one of the dimensionality reduction techniques.
- `.mute` a character vector containing the elements you want to mute (c("message", "output")), defaults to `character(0)`.
- `.keep.org.data` TRUE/FALSE keep the original data.

### Details

Method must be one of `dimRedMethodList()`, partial matching is performed. All parameters start with a dot, to avoid clashes with partial argument matching (see the R manual section 4.3.2), if there should ever occur any clashes in the arguments, call the function with all arguments named, e.g. `embed(.data = dat,.method = "mymethod", .d = "some parameter")`.

### Value

an object of class `dimRedResult`

### Methods (by class)

- `formula`: embed a data.frame using a formula.
- `ANY`: Embed anything as long as it can be coerced to `dimRedData`.
- `dimRedData`: Embed a dimRedData object

### Examples

```r
## embed a data.frame using a formula:

as.data.frame(
    embed(Species ~ Sepal.Length + Sepal.Width + Petal.Length + Petal.Width, iris, "PCA")
)
```
## embed a data.frame and return a data.frame
as.data.frame(embed(iris[, 1:4], "PCA"))

## embed a matrix and return a data.frame
as.data.frame(embed(as.matrix(iris[, 1:4]), "PCA"))

## Not run:
## embed dimRedData objects
embed_methods <- dimRedMethodList()
quality_methods <- dimRedQualityList()
dataset <- loadDataSet("Iris")

quality_results <- matrix(NA, length(embed_methods), length(quality_methods),
                          dimnames = list(embed_methods, quality_methods))
embedded_data <- list()

for (e in embed_methods) {
  message("embedding: ", e)
  embedded_data[[e]] <- embed(dataset, e, .mute = c("message", "output"))
  for (q in quality_methods) {
    message(" quality: ", q)
    quality_results[e, q] <- tryCatch(
      quality(embedded_data[[e]], q),
      error = function(e) NA
    )
  }
}

print(quality_results)

## End(Not run)

---

**FastICA-class**

**Independent Component Analysis**

**Description**

An S4 Class implementing the FastICA algorithm for Independent Component Analysis.

**Details**

ICA is used for blind signal separation of different sources. It is a linear Projection.

**Slots**

- **fun**: A function that does the embedding and returns a dimRedResult object.
- **stdpars**: The standard parameters for the function.
FruchtermanReingold-class

General usage

Dimensionality reduction methods are S4 Classes that either be used directly, in which case they have to be initialized and a full list with parameters has to be handed to the @fun() slot, or the method name be passed to the embed function and parameters can be given to the . . ., in which case missing parameters will be replaced by the ones in the @stdpars.

Parameters

FastICA can take the following parameters:

- **ndim** The number of output dimensions. Defaults to 2

Implementation

Wraps around fastICA. FastICA uses a very fast approximation for negentropy to estimate statistical independences between signals. Because it is a simple rotation/projection, forward and backward functions can be given.

References

Hyvarinen, A., 1999. Fast and robust fixed-point algorithms for independent component analysis. IEEE Transactions on Neural Networks 10, 626-634. https://doi.org/10.1109/72.761722

See Also

Other dimensionality reduction methods: AutoEncoder-class, DRR-class, DiffusionMaps-class, DrL-class, FruchtermanReingold-class, HLLE-class, Isomap-class, KamadaKawai-class, MDS-class, NNMF-class, PCA-class, PCA_L1-class, UMAP-class, dimRedMethod-class, dimRedMethodList(), kPCA-class, nMDS-class, tSNE-class

Examples

```r
if(requireNamespace("fastICA", quietly = TRUE)) {
  dat <- loadDataSet("3D S Curve")
  emb <- embed(dat, "FastICA", ndim = 2)
  plot(getData(getDimRedData(emb)))
}
```

FruchtermanReingold-class

*Fruchterman Reingold Graph Layout*

Description

An S4 Class implementing the Fruchterman Reingold Graph Layout algorithm.
Slots

fun A function that does the embedding and returns a dimRedResult object.

stdpars The standard parameters for the function.

General usage

Dimensionality reduction methods are S4 Classes that either be used directly, in which case they have to be initialized and a full list with parameters has to be handed to the @fun() slot, or the method name be passed to the embed function and parameters can be given to the . . . , in which case missing parameters will be replaced by the ones in the @stdpars.

Parameters

ndim The number of dimensions, defaults to 2. Can only be 2 or 3

knn Reduce the graph to keep only the nearest neighbors. Defaults to 100.

d The distance function to determine the weights of the graph edges. Defaults to euclidean distances.

Implementation

Wraps around layout_with_fr, see there for details. The Fruchterman Reingold algorithm puts the data into a circle and puts connected points close to each other.

References


See Also

Other dimensionality reduction methods: AutoEncoder-class, DRR-class, DiffusionMaps-class, DrL-class, FastICA-class, HLLE-class, Isomap-class, KamadaKawai-class, MDS-class, NNMF-class, PCA-class, PCA_L1-class, UMAP-class, dimRedMethod-class, dimRedMethodList(), kPCA-class, nMDS-class, tSNE-class

Examples

if(requireNamespace(c("igraph", "coRanking"), quietly = TRUE)) {

dat <- loadDataSet("Swiss Roll", n = 100)
emb <- embed(dat, "FruchtermanReingold")
plot(emb, type = "2vars")
}

**getData**

*Method getData*

**Description**

Extracts the data slot.

**Usage**

```r
data(object)
```

**Arguments**

- `object` The object to be converted.

**getDimRedData**

*Method getDimRedData*

**Description**

Extract dimRedData.

**Usage**

```r
data(object, ...)
```

**Arguments**

- `object` The object to extract data from.
  - `...` other arguments.

**getMeta**

*Method getMeta*

**Description**

Extracts the meta slot.

**Usage**

```r
meta(object, ...)
```

**Arguments**

- `object` The object to be converted.
  - `...` other arguments.
getNDim

Method getNDim

Description
Extract the number of embedding dimensions.

Usage
getNDim(object, ...)

Arguments

object The object to get the dimensions from.
... other arguments.

getOrgData

Method getOrgData

Description
Extract the Original data.

Usage
getOrgData(object, ...)

Arguments

object The object to extract data from.
... other arguments.

getOtherData

Method getOtherData

Description
Extract other data produced by a dimRedMethod.

Usage
getOtherData(object, ...)

Arguments

object The object to extract data from.
... other arguments.
**Method getPars**

**Description**
Extracts the pars slot.

**Usage**
getPars(object, ...)

**Arguments**
- **object**: The object to be converted.
- **...**: other arguments.

---

**getRotationMatrix**

**Description**
Extract the rotation matrix from dimRedResult objects derived from PCA and FastICA.

**Usage**
getRotationMatrix(x)

**Arguments**
- **x**: of type dimRedResult

**Details**
The data has to be pre-processed the same way as the method does, e.g. centering and/or scaling.

**Value**
a matrix
Examples

dat <- loadDataSet("Iris")

pca <- embed(dat, "PCA")
rot_pca <- getRotationMatrix(pca)
scale(getData(dat), TRUE, FALSE) \times rot_pca - getData(getDimRedData(pca))

if(requireNamespace("fastICA", quietly = TRUE)) {
  ica <- embed(dat, "FastICA")
  rot_ica <- getRotationMatrix(ica)
  scale(getData(dat), TRUE, FALSE) \times rot_ica - getData(getDimRedData(ica))
}

== HLLE-class ==

**Hessian Locally Linear Embedding**

Description

An S4 Class implementing Hessian Locally Linear Embedding (HLLE)

Details

HLLE uses local hessians to approximate the curvines and is an extension to non-convex subsets in lowdimensional space.

Slots

fun A function that does the embedding and returns a dimRedResult object.
stdpars The standard parameters for the function.

General usage

Dimensionality reduction methods are S4 Classes that either be used directly, in which case they have to be initialized and a full list with parameters has to be handed to the @fun() slot, or the method name be passed to the embed function and parameters can be given to the ..., in which case missing parameters will be replaced by the ones in the @stdpars.

Parameters

HLLE can take the following parameters:

knn neighborhood size
ndim number of output dimensions
Implementation

Own implementation, sticks to the algorithm in Donoho and Grimes (2003). Makes use of sparsity to speed up final embedding.

References


See Also

Other dimensionality reduction methods: AutoEncoder-class, DRR-class, DiffusionMaps-class, DrL-class, FastICA-class, FruchtermanReingold-class, Isomap-class, KamadaKawai-class, MDS-class, NNMF-class, PCA-class, PCA_L1-class, UMAP-class, dimRedMethod-class, dimRedMethodList(), kPCA-class, mDS-class, tSNE-class

Examples

```r
if(requireNamespace(c("RSpectra", "Matrix", "RANN"), quietly = TRUE)) {

  dat <- loadDataSet("3D S Curve", n = 300)
  emb <- embed(dat, "HLLE", knn = 15)
  plot(emb, type = "2vars")
}
```

installSuggests

Install packages which are suggested by dimRed.

Usage

installSuggests(...)

Arguments

... additional options passed to install.packages.

Details

By default dimRed will not install all the dependencies, because there are quite a lot and in case some of them are not available for your platform you will not be able to install dimRed without problems.

To solve this I provide a function which automatically installs all the suggested packages.
Examples

## Not run:
installSuggests()

## End(Not run)

Isomap-class  Isomap embedding

Description

An S4 Class implementing the Isomap Algorithm

Details

The Isomap algorithm approximates a manifold using geodesic distances on a k nearest neighbor graph. Then classical scaling is performed on the resulting distance matrix.

Slots

fun A function that does the embedding and returns a dimRedResult object.
stdpars The standard parameters for the function.

General usage

Dimensionality reduction methods are S4 Classes that either be used directly, in which case they have to be initialized and a full list with parameters has to be handed to the @fun() slot, or the method name be passed to the embed function and parameters can be given to the . . . , in which case missing parameters will be replaced by the ones in the @stdpars.

Parameters

Isomap can take the following parameters:

knn The number of nearest neighbors in the graph. Defaults to 50.
ndim The number of embedding dimensions, defaults to 2.
get_geod Should the geodesic distance matrix be kept, if TRUE, access it as getOtherData(x)$geod

Implementation

The dimRed package uses its own implementation of Isomap which also comes with an out of sample extension (known as landmark Isomap). The default Isomap algorithm scales computationally not very well, the implementation here uses nn2 for a faster search of the nearest neighbors. If data are too large it may be useful to fit a subsample of the data and use the out-of-sample extension for the other points.
References


See Also

Other dimensionality reduction methods: AutoEncoder-class, DRR-class, DiffusionMaps-class, DrL-class, FastICA-class, FruchtermanReingold-class, HLLE-class, KamadaKawai-class, MDS-class, NNMF-class, PCA-class, PCA_L1-class, UMAP-class, dimRedMethod-class, dimRedMethodList(), kPCA-class, nMDS-class, tSNE-class

Examples

```r
if(requireNamespace(c("RSpectra", "igraph", "RANN"), quietly = TRUE)) {
  dat <- loadDataSet("3D S Curve", n = 500)
  emb <- embed(dat, "Isomap", knn = 10)
  plot(emb)

  ## or simpler, use embed():
  samp <- sample(nrow(dat), size = 200)
  emb2 <- embed(dat[samp], "Isomap", .mute = NULL, knn = 10)
  emb3 <- predict(emb2, dat[-samp])

  plot(emb2, type = "2vars")
  plot(emb3, type = "2vars")
}
```

KamadaKawai-class

Graph Embedding via the Kamada Kawai Algorithm

Description

An S4 Class implementing the Kamada Kawai Algorithm for graph embedding.

Details

Graph embedding algorithms see the data as a graph. Between the nodes of the graph exist attracting and repelling forces which can be modeled as electrical fields or springs connecting the nodes. The graph is then forced into a lower dimensional representation that tries to represent the forces between the nodes accurately by minimizing the total energy of the attracting and repelling forces.

Slots

- `fun` A function that does the embedding and returns a dimRedResult object.
- `stdpars` The standard parameters for the function.
**General usage**

Dimensionality reduction methods are S4 Classes that either be used directly, in which case they have to be initialized and a full list with parameters has to be handed to the `@fun()` slot, or the method name be passed to the embed function and parameters can be given to the `. . .`, in which case missing parameters will be replaced by the ones in the `@stdpars`.

**Parameters**

KamadaKawai can take the following parameters:

- **ndim**  The number of dimensions, defaults to 2. Can only be 2 or 3
- **knn**  Reduce the graph to keep only the nearest neighbors. Defaults to 100.
- **d**  The distance function to determine the weights of the graph edges. Defaults to euclidean distances.

**Implementation**

Wraps around `layout_with_kk`. The parameters maxiter, epsilon and kkconst are set to the default values and cannot be set, this may change in a future release. The DimRed Package adds an extra sparsity parameter by constructing a knn graph which also may improve visualization quality.

**References**


**See Also**

Other dimensionality reduction methods: `AutoEncoder-class`, `DRR-class`, `DiffusionMaps-class`, `DrL-class`, `FastICA-class`, `FruchtermanReingold-class`, `HLLE-class`, `Isomap-class`, `MDS-class`, `NNMF-class`, `PCA-class`, `PCA_L1-class`, `UMAP-class`, `dimRedMethod-class`, `dimRedMethodList()`, `kPCA-class`, `nMDS-class`, `tSNE-class`

**Examples**

```r
if(requireNamespace(c("igraph", "coRanking"), quietly = TRUE)) {

dat <- loadDataSet("Swiss Roll", n = 200)
emb <- embed(dat, "KamadaKawai")
plot(emb, type = "2vars")

}
```
kPCA-class

Kernel PCA

Description
An S4 Class implementing Kernel PCA

Details
Kernel PCA is a nonlinear extension of PCA using kernel methods.

Slots
fun  A function that does the embedding and returns a dimRedResult object.
stdpars The standard parameters for the function.

General usage
Dimensionality reduction methods are S4 Classes that either be used directly, in which case they have to be initialized and a full list with parameters has to be handed to the @fun() slot, or the method name be passed to the embed function and parameters can be given to the ..., in which case missing parameters will be replaced by the ones in the @stdpars.

Parameters
Kernel PCA can take the following parameters:

ndim  the number of output dimensions, defaults to 2
kernel The kernel function, either as a function or a character vector with the name of the kernel. Defaults to "rbfdot"
kpar A list with the parameters for the kernel function, defaults to list(sigma = 0.1)

The most comprehensive collection of kernel functions can be found in kpca. In case the function does not take any parameters kpar has to be an empty list.

Implementation
Wraps around kpca, but provides additionally forward and backward projections.

References
LaplacianEigenmaps-class

See Also

Other dimensionality reduction methods: AutoEncoder-class, DRR-class, DiffusionMaps-class, DrL-class, FastICA-class, FruchtermanReingold-class, HLLE-class, Isomap-class, KamadaKawai-class, MDS-class, NNMF-class, PCA-class, PCA_L1-class, UMAP-class, dimRedMethod-class, dimRedMethodList(), nMDS-class, tsNE-class

Examples

## Not run:
if(requireNamespace("kernlab", quietly = TRUE)) {

dat <- loadDataSet("3D S Curve")
emb <- embed(dat, "kPCA")
plot(emb, type = "2vars")
}

## End(Not run)

LaplacianEigenmaps-class

Laplacian Eigenmaps

Description

An S4 Class implementing Laplacian Eigenmaps

Details

Laplacian Eigenmaps use a kernel and were originally developed to separate non-convex clusters under the name spectral clustering.

Slots

fun A function that does the embedding and returns a dimRedResult object.
stdpars The standard parameters for the function.

General usage

Dimensionality reduction methods are S4 Classes that either be used directly, in which case they have to be initialized and a full list with parameters has to be handed to the @fun() slot, or the method name be passed to the embed function and parameters can be given to the . . ., in which case missing parameters will be replaced by the ones in the @stdpars.
Parameters

LaplacianEigenmaps can take the following parameters:

- **ndim** the number of output dimensions.
- **sparse** A character vector specifying how to make the graph sparse, "knn" means that a K-nearest neighbor graph is constructed, "eps" an epsilon neighborhood graph is constructed, else a dense distance matrix is used.
- **knn** The number of nearest neighbors to use for the knn graph.
- **eps** The distance for the epsilon neighborhood graph.
- **t** Parameter for the transformation of the distance matrix by $w = \exp(-d^2/t)$, larger values give less weight to differences in distance, $t = \infty$ treats all distances $\neq 0$ equally.
- **norm** logical, should the normed laplacian be used?

Implementation

Wraps around `spec.emb`.

References


Examples

```r
if(requireNamespace(c("loe", "RSpectra", "Matrix"), quietly = TRUE)) {
  dat <- loadDataSet("3D S Curve")
  emb <- embed(dat, "LaplacianEigenmaps")
  plot(emb@data@data)
}
```

LCMC, dimRedResult-method

**Method LCMC**

Description

Calculates the Local Continuity Meta Criterion, which is $Q_{NX}$ adjusted for random overlap inside the K-ary neighborhood.

Usage

```r
## S4 method for signature 'dimRedResult'
LCMC(object)
```
makeKNNgraph

Arguments

object of class dimRedResult

See Also


Description

Create a K-nearest neighbor graph from data x. Uses nn2 as a fast way to find the nearest neighbors.

Usage

makeKNNgraph(x, k, eps = 0, diag = FALSE)

Arguments

x data, a matrix, observations in rows, dimensions in columns
k the number of nearest neighbors.
eps number, if eps > 0 the KNN search is approximate, see nn2
diag logical, if TRUE every edge of the returned graph will have an edge with weight 0 to itself.

Value

an object of type igraph with edge weight being the distances.
maximize_correlation, dimRedResult-method

Maximize Correlation with the Axes

Description

Rotates the data in such a way that the correlation with the first naxes axes is maximized.

Usage

```r
## S4 method for signature 'dimRedResult'
maximize_correlation(
  object,
  naxes = ncol(object@data@data),
  cor_method = "pearson"
)
```

Arguments

- `object`: A dimRedResult object
- `naxes`: the number of axes to optimize for.
- `cor_method`: which correlation method to use

Details

Methods that do not use eigenvector decomposition, like t-SNE often do not align the data with axes according to the correlation of variables with the data. maximize_correlation uses the optimx package to rotate the data in such a way that the original variables have maximum correlation with the embedding axes.

MDS-class

Metric Dimensional Scaling

Description

An S4 Class implementing classical scaling (MDS).

Details

MDS tries to maintain distances in high- and low-dimensional space, it has the advantage over PCA that arbitrary distance functions can be used, but it is computationally more demanding.

Slots

- `fun`: A function that does the embedding and returns a dimRedResult object.
- `stdpars`: The standard parameters for the function.
General usage

Dimensionality reduction methods are S4 Classes that either be used directly, in which case they have to be initialized and a full list with parameters has to be handed to the @fun() slot, or the method name be passed to the embed function and parameters can be given to the ... in which case missing parameters will be replaced by the ones in the @stdpars.

Parameters

MDS can take the following parameters:

\textbf{ndim} The number of dimensions.

\textbf{d} The function to calculate the distance matrix from the input coordinates, defaults to euclidean distances.

Implementation

Wraps around \texttt{cmdscale}. The implementation also provides an out-of-sample extension which is not completely optimized yet.

References


See Also

Other dimensionality reduction methods: \texttt{AutoEncoder-class}, \texttt{DRR-class}, \texttt{DiffusionMaps-class}, \texttt{DrL-class}, \texttt{FastICA-class}, \texttt{FruchtermanReingold-class}, \texttt{HLLE-class}, \texttt{Isomap-class}, \texttt{KamadaKawai-class}, \texttt{NNMF-class}, \texttt{PCA-class}, \texttt{PCA_L1-class}, \texttt{UMAP-class}, \texttt{dimRedMethod-class}, \texttt{dimRedMethodList()}, \texttt{kPCA-class}, \texttt{nMDS-class}, \texttt{tSNE-class}

Examples

```r
# Not run:
dat <- loadDataSet("3D S Curve")
emb <- embed(dat, "MDS")
plot(emb, type = "2vars")

# a "manual" kPCA:
emb2 <- embed(dat, "MDS", d = function(x) exp(stats::dist(x)))
plot(emb2, type = "2vars")

# a "manual", more customizable, and slower Isomap:
emb3 <- embed(dat, "MDS", d = function(x) vegan::isomapdist(vegan::vegdist(x, "manhattan"), k = 20))
plot(emb3)

# End(Not run)
```
### mean_R_NX, dimRedResult-method

**Method mean_R_NX**

#### Description

Calculate the mean_R_NX score to assess the quality of a dimensionality reduction.

#### Usage

```r
## S4 method for signature 'dimRedResult'
mean_R_NX(object)
```

#### Arguments

- `object` of class `dimRedResult`

#### See Also


---

### mixColorRamps

**Mixing color ramps**

#### Description

mix different color ramps

#### Usage

```r
mixColorRamps(vars, ramps)
mixColor1Ramps(vars, ramps = colorRamp(c("blue", "black", "red")))
mixColor2Ramps(
  vars,
  ramps = list(colorRamp(c("blue", "green")), colorRamp(c("blue", "red")))
)
mixColor3Ramps(
  vars,
  ramps = list(colorRamp(c("#001A00", "#00E600")), colorRamp(c("#00001A", "#0000E6")),
                colorRamp(c("#1A0000", "#E60000")))
)
```
**Arguments**

- **vars**: a list of variables
- **ramps**: a list of color ramps, one for each variable.

**Details**

automatically create colors to represent a varying number of dimensions.

**Examples**

```r
cols <- expand.grid(x = seq(0, 1, length.out = 10),
                    y = seq(0, 1, length.out = 10),
                    z = seq(0, 1, length.out = 10))
mixed <- mixColor3Ramps(cols)

# Not run:
if(requireNamespace("rgl", quietly = TRUE)) {
  rgl::plot3d(cols$x, cols$y, cols$z, col = mixed, pch = 15)
}

cols <- expand.grid(x = seq(0, 1, length.out = 10),
                    y = seq(0, 1, length.out = 10))
mixed <- mixColor2Ramps(cols)

if(requireNamespace("graphics", quietly = TRUE)) {
  plot(cols$x, cols$y, col = mixed, pch = 15)
}

# End(Not run)
```

---

**ndims Method**

**Description**

Extract the number of dimensions.

**Usage**

```r
ndims(object, ...)
```

**Arguments**

- **object**: To extract the number of dimensions from.
- **...**: Arguments for further methods
nMDS-class

Non-Metric Dimensional Scaling

Description

An S4 Class implementing Non-Metric Dimensional Scaling.

Details

A non-linear extension of MDS using monotonic regression

Slots

fun A function that does the embedding and returns a dimRedResult object.
stdpars The standard parameters for the function.

General usage

Dimensionality reduction methods are S4 Classes that either be used directly, in which case they have to be initialized and a full list with parameters has to be handed to the @fun() slot, or the method name be passed to the embed function and parameters can be given to the . . . , in which case missing parameters will be replaced by the ones in the @stdpars.

Parameters

nMDS can take the following parameters:

- d A distance function.
- ndim The number of embedding dimensions.

Implementation

Wraps around the monoMDS. For parameters that are not available here, the standard configuration is used.

References


See Also

Other dimensionality reduction methods: AutoEncoder-class, DRR-class, DiffusionMaps-class, DrL-class, FastICA-class, FruchtermanReingold-class, HLLE-class, Isomap-class, KamadaKawai-class, MDS-class, NNMF-class, PCA-class, PCA_L1-class, UMAP-class, dimRedMethod-class, dimRedMethodList(), kPCA-class, tSNE-class
Examples

if(requireNamespace("vegan", quietly = TRUE)) {

dat <- loadDataSet("3D S Curve", n = 300)
emb <- embed(dat, "nMDS")
plot(emb, type = "2vars")
}

NNMF-class

Non-Negative Matrix Factorization

Description

S4 Class implementing NNMF.

Details

NNMF is a method for decomposing a matrix into a smaller dimension such that the constraint that the data (and the projection) are not negative is taken into account.

Slots

fun A function that does the embedding and returns a dimRedResult object.
stdpars The standard parameters for the function.

General usage

Dimensionality reduction methods are S4 Classes that either be used directly, in which case they have to be initialized and a full list with parameters has to be handed to the @fun() slot, or the method name be passed to the embed function and parameters can be given to the . . . , in which case missing parameters will be replaced by the ones in the @stdpars.

Parameters

The method can take the following parameters:

ndim The number of output dimensions.
method character, which algorithm should be used. See nmf for possible values. Defaults to "brunet"
nrun integer, the number of times the computations are conducted. See nmf
seed integer, a value to control the random numbers used.
options named list, other options to pass to nmf
Implementation

Wraps around \texttt{nmf}. Note that the estimation uses random numbers. To create reproducible results, set the random number seed in the function call. Also, in many cases, the computations will be conducted in parallel using multiple cores. To disable this, use the option \texttt{.pbackend = NULL}.

References


See Also

Other dimensionality reduction methods: \texttt{AutoEncoder-class}, \texttt{DRR-class}, \texttt{DiffusionMaps-class}, \texttt{DrI-class}, \texttt{FastICA-class}, \texttt{FruchtermanReingold-class}, \texttt{HLLE-class}, \texttt{Isomap-class}, \texttt{KamadaKawai-class}, \texttt{MDS-class}, \texttt{PCA-class}, \texttt{PCA_L1-class}, \texttt{UMAP-class}, \texttt{dimRedMethod-class}, \texttt{dimRedMethodList()}, \texttt{kPCA-class}, \texttt{nMDS-class}, \texttt{tSNE-class}

Examples

if(requireNamespace(c("NNMF", "MASS"), quietly = TRUE)) {

  set.seed(4646)
  dat <- loadDataSet("Iris")
  emb <- embed(dat, "NNMF")

  plot(emb)

  # project new values:
  nn_proj <- predict(emb, dat[1:7])
  plot(nn_proj)

}

PCA-class

\textit{Principal Component Analysis}

Description

S4 Class implementing PCA.

Details

PCA transforms the data in orthogonal components so that the first axis accounts for the largest variance in the data, all the following axes account for the highest variance under the constraint that they are orthogonal to the preceding axes. PCA is sensitive to the scaling of the variables. PCA is by far the fastest and simplest method of dimensionality reduction and should probably always be applied as a baseline if other methods are tested.
Slots

fun  A function that does the embedding and returns a dimRedResult object.

stdpars  The standard parameters for the function.

General usage

Dimensionality reduction methods are S4 Classes that either be used directly, in which case they
have to be initialized and a full list with parameters has to be handed to the @fun() slot, or the
method name be passed to the embed function and parameters can be given to the . . . , in which
case missing parameters will be replaced by the ones in the @stdpars.

Parameters

PCA can take the following parameters:

ndim  The number of output dimensions.

center  logical, should the data be centered, defaults to TRUE.

scale.  logical, should the data be scaled, defaults to FALSE.

Implementation

Wraps around prcomp. Because PCA can be reduced to a simple rotation, forward and backward
projection functions are supplied.

References

Pearson, K., 1901. On lines and planes of closest fit to systems of points in space. Philosophical
Magazine 2, 559-572.

See Also

Other dimensionality reduction methods: AutoEncoder-class, DRR-class, DiffusionMaps-class,
DrL-class, FastICA-class, FruchtermanReingold-class, HLLE-class, Isomap-class, KamadaKawai-class,
MDS-class, NNMF-class, PCA_L1-class, UMAP-class, dimRedMethod-class, dimRedMethodList(),
kPCA-class, nMDS-class, tSNE-class

Examples

dat <- loadDataSet("Iris")
emb <- embed(dat, "PCA")

plot(emb, type = "2vars")
if(requireNamespace("scatterplot3d", quietly = TRUE))
  plot(inverse(emb, getDimRedData(emb)), type = "3vars")
Description

S4 Class implementing PCA with L1 error.

Details

PCA transforms the data so that the L2 reconstruction error is minimized or the variance of the projected data is maximized. This is sensitive to outliers, L1 PCA minimizes the L1 reconstruction error or maximizes the sum of the L1 norm of the projected observations.

Slots

fun  A function that does the embedding and returns a dimRedResult object.
stdpars  The standard parameters for the function.

General usage

Dimensionality reduction methods are S4 Classes that either be used directly, in which case they have to be initialized and a full list with parameters has to be handed to the @fun() slot, or the method name be passed to the embed function and parameters can be given to the . . . , in which case missing parameters will be replaced by the ones in the @stdpars.

Parameters

PCA can take the following parameters:

ndim  The number of output dimensions.
center  logical, should the data be centered, defaults to TRUE.
scale.  logical, should the data be scaled, defaults to FALSE.
fun  character or function, the method to apply, see the pcaL1 package
...  other parameters for fun

Implementation

Wraps around the different methods is the pcaL1 package. Because PCA can be reduced to a simple rotation, forward and backward projection functions are supplied.

References

**plot**

### Description

Plots a object of class dimRedResult and dimRedData. For the documentation of the plotting function in base see here: `plot.default`.

### Usage

```r
plot(x, y, ...)  
```

**Examples**

```r
if(requireNamespace("pcaL1", quietly = TRUE)) {
  dat <- loadDataSet("Iris")
  emb <- embed(dat, "PCA_L1")
  plot(emb, type = "2vars")
  plot(inverse(emb, getData(getDimRedData((emb)))), type = "3vars")
}
```

### See Also

Other dimensionality reduction methods: **AutoEncoder-class**, **DRR-class**, **DiffusionMaps-class**, **DrL-class**, **FastICA-class**, **FruchtermanReingold-class**, **HLLE-class**, **Isomap-class**, **KamadaKawai-class**, **MDS-class**, **NNMF-class**, **PCA-class**, **UMAP-class**, **dimRedMethod-class**, **dimRedMethodList()**, **kPCA-class**, **nMDS-class**, **tSNE-class**

---

**plot**

*Plotting of dimRed* objects

---

**Description**

Plots a object of class dimRedResult and dimRedData. For the documentation of the plotting function in base see here: `plot.default`.

**Usage**

```r
plot(x, y, ...)  
```

### Examples

```r
if(requireNamespace("pcaL1", quietly = TRUE)) {
  dat <- loadDataSet("Iris")
  emb <- embed(dat, "PCA_L1")
  plot(emb, type = "2vars")
  plot(inverse(emb, getData(getDimRedData((emb)))), type = "3vars")
}
```
Arguments

- **x**: dimRedResult/dimRedData class, e.g. output of embedded/loadDataSet
- **y**: Ignored
- **type**: plot type, one of c("pairs", "parpl", "2vars", "3vars", "3varsrgl")
- **vars**: the axes of the embedding to use for plotting
- **col**: the columns of the meta slot to use for coloring, can be referenced as the column names or number of x@data

Details

Plotting functions for the classes usind in dimRed. They are intended to give a quick overview over the results, so they are somewhat inflexible, e.g. it is hard to modify color scales or plotting parameters.

If you require more control over plotting, it is better to convert the object to a data.frame first and use the standard functions for plotting.

Methods (by class)

- **x = dimRedData, y = ANY**: Ploting of dimRedData objects
- **x = dimRedResult, y = ANY**: Ploting of dimRedResult objects.

Examples

```r
scurve = loadDataSet("3D S Curve")
if(requireNamespace("graphics", quietly = TRUE))
  plot(scurve, type = "pairs", main = "pairs plot of S curve")
if(requireNamespace("MASS", quietly = TRUE))
  plot(scurve, type = "parpl")
if(requireNamespace("graphics", quietly = TRUE))
  plot(scurve, type = "2vars", vars = c("y", "z"))
if(requireNamespace("scatterplot3d", quietly = TRUE))
  plot(scurve, type = "3vars")
if(requireNamespace("rgl", quietly = TRUE))
  plot(scurve, type = "3varsrgl")
```

Description

Plot the R_NX curve for different embeddings. Takes a list of dimRedResult objects as input. Also the Area under the curve values are computed for a weighted K (see AUC_InK_R_NX for details) and appear in the legend.
Usage

plot_R_NX(x, ndim = NA, weight = "inv")

Arguments

x  
a list of dimRedResult objects. The names of the list will appear in the legend with the AUC_InK value.

ndim  
the number of dimensions, if NA the original number of embedding dimensions is used, can be a vector giving the embedding dimensionality for each single list element of x.

weight  
the weight function used for K when calculating the AUC, one of c("inv", "log", "log10")

Value

A ggplot object, the design can be changed by appending theme(…)

See Also


Examples

if(requireNamespace(c("RSpectra", "igraph", "RANN", "ggplot", "tidyr", "scales"), quietly = TRUE)) {
  ## define which methods to apply
  embed_methods <- c("Isomap", "PCA")
  ## load test data set
  data_set <- loadDataSet("3D S Curve", n = 200)
  ## apply dimensionality reduction
  data_emb <- lapply(embed_methods, function(x) embed(data_set, x))
  names(data_emb) <- embed_methods
  ## plot the R_NX curves:
  plot_R_NX(data_emb) +
    ggplot2::theme(legend.title = ggplot2::element_blank(),
                   legend.position = c(0.5, 0.1),
                   legend.justification = c(0.5, 0.1))
}
**print**

*Method print*

**Description**
Imports the print method into the package namespace.

**Usage**

```r
print(x, ...)
```

**Arguments**

- `x` The object to be printed.
- `...` Other arguments for printing.

**quality, dimRedResult-method**

*Quality Criteria for dimensionality reduction.*

**Description**
A collection of functions to compute quality measures on `dimRedResult` objects.

**Usage**

```r
## S4 method for signature 'dimRedResult'
quality(.data, .method = dimRedQualityList(), .mute = character(0), ...)

dimRedQualityList(filter = FALSE)
```

**Arguments**

- `.data` object of class `dimRedResult`
- `.method` character vector naming one of the methods
- `.mute` what output from the embedding method should be muted.
- `...` the parameters, internally passed as a list to the quality method as `pars = list(...)`
- `filter` filter methods by installed packages

**Value**

a number
Methods (by class)

• dimRedResult: Calculate a quality index from a dimRedResult object.

Implemented methods

Method must be one of "Q_local", "Q_global", "mean_R_NX", "total_correlation", "cophenetic_correlation", "distance_correlation", "reconstruction_rmse"

Rank based criteria

Q_local, Q_global, and mean_R_NX are quality criteria based on the Co-ranking matrix. Q_local and Q_global determine the local/global quality of the embedding, while mean_R_NX determines the quality of the overall embedding. They are parameter free and return a single number. The object must include the original data. The number returns is in the range [0, 1], higher values mean a better local/global embedding.

Correlation based criteria

total_correlation calculates the sum of the mean squared correlations of the original axes with the axes in reduced dimensions, because some methods do not care about correlations with axes, there is an option to rotate data in reduced space to maximize this criterion. The number may be greater than one if more dimensions are summed up.

cophenetic_correlation calculate the correlation between the lower triangles of distance matrices, the correlation and distance methods may be specified. The result is in range [-1, 1].

distance_correlation measures the independencies of samples by calculating the correlation of distances. For details see dcor.

Reconstruction error

reconstruction_rmse calculates the root mean squared error of the reconstruction. object requires an inverse function.

Author(s)

Guido Kraemer

References


See Also


Examples

## Not run:
embed_methods <- dimRedMethodList()
quality_methods <- dimRedQualityList()
scurve <- loadDataSet("Iris")

quality_results <- matrix(NA, length(embed_methods), length(quality_methods),
dimnames = list(embed_methods, quality_methods))
embedded_data <- list()

for (e in embed_methods) {
  message("embedding: ", e)
  embedded_data[[e]] <- embed(scurve, e, .mute = c("message", "output"))
  for (q in quality_methods) {
    message(" quality: ", q)
    quality_results[e, q] <- tryCatch(
      quality(embedded_data[[e]], q),
      error = function (e) NA
    )
  }
}

print(quality_results)

## End(Not run)

---

**Q_global**

**Method Q_global**

**Description**

Calculate the Q_global score to assess the quality of a dimensionality reduction.

**Usage**

```r
## S4 method for signature 'dimRedResult'
Q_global(object)
```

**Arguments**

- `object` of class `dimRedResult`
See Also


---

**Method Q\_local**

**Description**

Calculate the Q\_local score to assess the quality of a dimensionality reduction.

**Usage**

```r
## S4 method for signature 'dimRedResult'
Q\_local(object, ndim = getNDim(object))
```

**Arguments**

- `object`: of class `dimRedResult`.
- `ndim`: use the first `ndim` columns of the embedded data for calculation.

**See Also**


---

**Method Q\_NX**

**Description**

Calculate the Q\_NX score (Chen & Buja 2006, the notation in the publication is M\_k). Which is the fraction of points that remain inside the same K-ary neighborhood in high and low dimensional space.
reconstruction_error.dimRedResult-method

Usage

```r
## S4 method for signature 'dimRedResult'
Q_NX(object)
```

Arguments

- `object` of class `dimRedResult`

See Also


---

reconstruction_error, dimRedResult-method

*Method reconstruction_error*

Description

Calculate the error using only the first $n$ dimensions of the embedded data. `error_fun` can either be one of c("rmse", "mae") to calculate the root mean square error or the mean absolute error respectively, or a function that takes to equally sized vectors as input and returns a single number as output.

Usage

```r
## S4 method for signature 'dimRedResult'
reconstruction_error(object, n = seq_len(ndims(object)), error_fun = "rmse")
```

Arguments

- `object` of class `dimRedResult`
- `n` a positive integer or vector of integers $\leq$ ndims(object)
- `error_fun` a function or string indicating an error function, if indication a function it must take to matrices of the same size and return a scalar.

Value

- a vector of number with the same length as $n$ with the

Author(s)

Guido Kraemer
See Also


Examples

```r
## Not run:
ir <- loadDataSet("Iris")
ir.drr <- embed(ir, "DRR", ndim = ndims(ir))
ir.pca <- embed(ir, "PCA", ndim = ndims(ir))

rmse <- data.frame(
  rmse_drr = reconstruction\_error(ir.drr),
  rmse_pca = reconstruction\_error(ir.pca)
)

matplot(rmse, type = "l")
plot(ir)
plot(ir.drr)
plot(ir.pca)

## End(Not run)
```

---

### Method reconstruction\_rmse

**Description**

Calculate the reconstruction root mean squared error a dimensionality reduction, the method must have an inverse mapping.

**Usage**

```r
## S4 method for signature 'dimRedResult'
reconstruction\_rmse(object)
```

**Arguments**

- `object` of class dimRedResult
Method R_NX

Description
Calculate the R_NX score from Lee et. al. (2013) which shows the neighborhood preservation for the Kth nearest neighbors, corrected for random point distributions and scaled to range [0, 1].

Usage
```r
## S4 method for signature 'dimRedResult'
R_NX(object, ndim = getNDim(object))
```

Arguments
- `object`: of class dimRedResult
- `ndim`: the number of dimensions to take from the embedded data.

See Also
Other Quality scores for dimensionality reduction:

Method total_correlation

Description
Calculate the total correlation of the variables with the axes to assess the quality of a dimensionality reduction.
Usage

## S4 method for signature 'dimRedResult'
total_correlation(
  object,
  naxes = ndims(object),
  cor_method = "pearson",
  is.rotated = FALSE
)

Arguments

- **object** of class dimRedResult
- **naxes** the number of axes to use for optimization.
- **cor_method** the correlation method to use.
- **is.rotated** if FALSE the object is rotated.

See Also


---

### tSNE-class

**t-Distributed Stochastic Neighborhood Embedding**

**Description**

An S4 Class for t-SNE.

**Details**

t-SNE is a method that uses Kullback-Leibler divergence between the distance matrices in high and low-dimensional space to embed the data. The method is very well suited to visualize complex structures in low dimensions.

**Slots**

- **fun** A function that does the embedding and returns a dimRedResult object.
- **stdpars** The standard parameters for the function.

**General usage**

Dimensionality reduction methods are S4 Classes that either be used directly, in which case they have to be initialized and a full list with parameters has to be handed to the @fun() slot, or the method name be passed to the embed function and parameters can be given to the ... in which case missing parameters will be replaced by the ones in the @stdpars.
Parameters

- **t-SNE** can take the following parameters:
  - `d` A distance function, defaults to euclidean distances
  - **perplexity** The perplexity parameter, roughly equivalent to neighborhood size.
  - **theta** Approximation for the nearest neighbour search, large values are more inaccurate.
  - **ndim** The number of embedding dimensions.

Implementation

Wraps around Rtsne, which is very well documented. Setting `theta = 0` does a normal t-SNE, larger values for `theta < 1` use the Barnes-Hut algorithm which scales much nicer with data size. Larger values for perplexity take larger neighborhoods into account.

References


See Also

Other dimensionality reduction methods: AutoEncoder-class, DRR-class, DiffusionMaps-class, DrL-class, FastICA-class, FruchtermanReingold-class, HLLE-class, Isomap-class, KamadaKawai-class, MDS-class, NNMF-class, PCA-class, PCA_L1-class, UMAP-class, dimRedMethod-class, dimRedMethodList(), kPCA-class, nMDS-class

Examples

```r
## Not run:
dat <- loadDataSet("3D S Curve", n = 300)
emb <- embed(dat, "tSNE", perplexity = 80)
plot(emb, type = "2vars")
## End(Not run)
```

**UMAP-class**

*Umap embedding*

Description

An S4 Class implementing the UMAP algorithm

Details

Uniform Manifold Approximation is a gradient descend based algorithm that gives results similar to t-SNE, but scales better with the number of points.
Slots

fun  A function that does the embedding and returns a dimRedResult object.
stdpars  The standard parameters for the function.

General usage

Dimensionality reduction methods are S4 Classes that either be used directly, in which case they have to be initialized and a full list with parameters has to be handed to the @fun() slot, or the method name be passed to the embed function and parameters can be given to the . . . , in which case missing parameters will be replaced by the ones in the @stdpars.

Parameters

UMAP can take the follwing parameters:

ndim  The number of embedding dimensions.
knn  The number of neighbors to be used.
d  The distance metric to use.
method  "naive" for an R implementation, "python" for the reference implementation.

Other method parameters can also be passed, see umap.defaults for details. The ones above have been standardized for the use with dimRed and will get automatically translated for umap.

Implementation

The dimRed package wraps the umap packages which provides an implementation in pure R and also a wrapper around the original python package umap-learn (https://github.com/lmcinnes/umap/). This requires umap-learn version 0.4 installed, at the time of writing, there is already umap-learn 0.5 but it is not supported by the R package umap.

The "naive" implementation is a pure R implementation and considered experimental at the point of writing this, it is also much slower than the python implementation.

The "python" implementation is the reference implementation used by McInees et. al. (2018). It requires the reticulate package for the interaction with python and the python package umap-learn installed (use pip install umap-learn).

References


See Also

Other dimensionality reduction methods: AutoEncoder-class, DRR-class, DiffusionMaps-class, DrL-class, FastICA-class, FruchtermanReingold-class, HLLE-class, Isomap-class, KamadaKawai-class, MDS-class, NNMF-class, PCA-class, PCA_L1-class, dimRedMethod-class, dimRedMethodList(), kPCA-class, nMDS-class, tSNE-class
Examples

```r
## Not run:
dat <- loadDataSet("3D S Curve", n = 300)
emb <- embed(dat, "UMAP", .mute = NULL, knn = 10)
plot(emb, type = "2vars")

## End(Not run)
```
Index

* Quality scores for dimensionality reduction
  AUC\_lnK\_R\_NX,\dimRedResult\text{-method}, 5
  cophenetic\_correlation,\dimRedResult\text{-method}, 8
  distance\_correlation,\dimRedResult\text{-method}, 17
  LCMC,\dimRedResult\text{-method}, 36
  mean\_R\_NX,\dimRedResult\text{-method}, 40
  plot\_R\_NX, 48
  Q\_global,\dimRedResult\text{-method}, 52
  Q\_local,\dimRedResult\text{-method}, 53
  Q\_NX,\dimRedResult\text{-method}, 53
  quality,\dimRedResult\text{-method}, 50
  R\_NX,\dimRedResult\text{-method}, 56
  reconstruction\_error,\dimRedResult\text{-method}, 54
  reconstruction\_rmse,\dimRedResult\text{-method}, 55
  total\_correlation,\dimRedResult\text{-method}, 56
* convenience functions
  getRotationMatrix, 28
* \dimRedData
  as.\dimRedData, 4
  \dimRedData\text{-class}, 11
* \dimRedResult
  \dimRedResult\text{-class}, 15
* dimensionality reduction methods
  AutoEncoder\text{-class}, 6
  DiffusionMaps\text{-class}, 10
  \dimRedMethod\text{-class}, 13
  \dimRedMethodList, 14
  Drl\text{-class}, 18
  DRR\text{-class}, 19
  FastICA\text{-class}, 23
  FruchtermanReingold\text{-class}, 24
  HLLE\text{-class}, 29
  Isomap\text{-class}, 31
  KamadaKawai\text{-class}, 32
  kPCA\text{-class}, 34
  MDS\text{-class}, 38
  nMDS\text{-class}, 42
  NNMF\text{-class}, 43
  PCA\text{-class}, 44
  PCA\_L1\text{-class}, 46
  tSNE\text{-class}, 57
  UMAP\text{-class}, 58
  [,\dimRedData,ANY,ANY,ANY\text{-method}
  \text{(dimRedData\text{-class}), 11
  as.\text{data.frame}, 4, 4
  as.\text{data.frame},\dimRedData\text{-method}
  \text{(dimRedData\text{-class}), 11
  as.\text{data.frame},\dimRedResult\text{-method}
  \text{(dimRedResult\text{-class}), 15
  as.\text{data.frame}.\text{default}, 4
  as.\dimRedData, 4, 12, 22
  as.\dimRedData,\text{formula\text{-method}
  \text{(as.\dimRedData), 4
  AUC\_lnK\_R\_NX, 48
  AUC\_lnK\_R\_NX
  \text{(AUC\_lnK\_R\_NX,\dimRedResult\text{-method), 5
  AUC\_lnK\_R\_NX,\dimRedResult\text{-method}, 5
  AutoEncoder\text{ (AutoEncoder\text{-class), 6
  AutoEncoder\text{-class, 6
  cmdscale, 39
  constructFastKRR\text{ Learner, 20
  constructKRR\text{ Learner, 20
  cophenetic\_correlation, 51
  cophenetic\_correlation
  \text{(cophenetic\_correlation,\dimRedResult\text{-method), 8
  cophenetic\_correlation,\dimRedResult\text{-method, 8
  data.\text{frame}, 4

61
datasetList ( dataSet ), 9
dataSets, 9
dcor, 51
diffuse, 10
DiffusionMaps ( DiffusionMaps-class ), 10
DiffusionMaps-class, 10
dimRed ( dimRed-package ), 3
dimRed-package, 3
dimRedData, 4, 9, 13, 16, 22
dimRedData ( dimRedData-class ), 11
dimRedData-class, 11
dimRedMethod-class, 13
dimRedMethodList, 7, 11, 14, 19, 20, 22, 24, 25, 30, 32, 33, 35, 39, 42, 44, 45, 47, 58, 59
dimRedQualityList
  ( quality, dimRedResult-method ), 50
dimRedResult, 4, 7, 14, 22, 28, 48–50
dimRedResult ( dimRedResult-class ), 15
dimRedResult-class, 15
dist, 10
distance_correlation, 51
distance_correlation
  ( distance_correlation, dimRedResult-method ), 17
distance_correlation, dimRedResult-method, 17
DrL ( DrL-class ), 18
DrL-class, 18
DRR ( DRR-class ), 19
drr, 20
DRR-class, 19

embed, 14, 21
embed, ANY-method ( embed ), 21
embed, dimRedData-method ( embed ), 21
embed, formula-method ( embed ), 21

fastCV, 20
FastICA ( FastICA-class ), 23
fastICA, 24
FastICA-class, 23
FruchtermanReingold
  ( FruchtermanReingold-class ), 24
FruchtermanReingold-class, 24

getData, 26
data, dimRedData-method
  ( dimRedData-method ), 11
dataDimRedData, 26
dataDimRedData, dimRedResult-method
  ( dimRedResult-class ), 15
dataMeta, 26
dataMeta, dimRedData-method
  ( dimRedData-class ), 11
getDataNDim, 27
dataNDim, dimRedResult-method
  ( dimRedResult-class ), 15
dataOrgData, 27
dataOrgData, dimRedResult-method
  ( dimRedResult-class ), 15
dataOtherData, 27
dataOtherData, dimRedResult-method
  ( dimRedResult-class ), 15
dataPars, 28
dataPars, dimRedResult-method
  ( dimRedResult-class ), 15
getDataRotationMatrix, 28

HLLE ( HLLE-class ), 29
HLLE-class, 29

igraph, 37
installSuggests, 30
inverse ( dimRedResult-class ), 15
inverse, dimRedResult-method
  ( dimRedResult-class ), 15
Isomap ( Isomap-class ), 31
Isomap-class, 31

KamadaKawai ( KamadaKawai-class ), 32
KamadaKawai-class, 32
kPCA ( kPCA-class ), 34
kpca, 34
kPCA-class, 34

LaplacianEigenmaps
  ( LaplacianEigenmaps-class ), 35
LaplacianEigenmaps-class, 35
layer_input, 7
layout_with_drl, 18
layout_with_fr, 25
layout_with_kk, 33
LCMC ( LCMC, dimRedResult-method ), 36
LCMC, dimRedResult-method, 36
loadDataSet ( dataSet ), 9
INDEX

makeKNNgraph, 37
match.arg, 9
maximize_correlation
  (maximize_correlation,dimRedResult-method), 38
maximize_correlation,dimRedResult-method, 38
MDS (MDS-class), 38
MDS-class, 38
mean_R_NX, 51
  (mean_R_NX,dimRedResult-method), 40
mean_R_NX, 40
mixColor1Ramps (mixColorRamps), 40
mixColor2Ramps (mixColorRamps), 40
mixColor3Ramps (mixColorRamps), 40
mixColorRamps, 40
monoMDS, 42
ndims, 41
  (ndims,dimRedData-method)
  (ndims,dimRedResult-method), 11
ndims, dimRedData-method
  (ndims,dimRedData-class), 11
ndims, dimRedResult-method
  (ndims,dimRedResult-class), 15
nMDS (nMDS-class), 42
nMDS-class, 42
nmf, 43, 44
nn2, 31, 37
NNMF (NNMF-class), 43
NNMF-class, 43
nrow, dimRedData-method
  (nrow,dimRedData-class), 11
optimx, 38
PCA (PCA-class), 44
PCA-class, 44
PCA_L1 (PCA_L1-class), 46
PCA_L1-class, 46
plot, 47
plot, dimRedData, ANY-method (plot), 47
plot, dimRedResult, ANY-method (plot), 47
plot.default, 47
plot (plot), 47
plot, dimRedData, 12
plot, dimRedData (plot), 47
plot, dimRedResult (plot), 47
plot_R_NX, 5, 8, 18, 37, 40, 48, 52–57
prcomp, 45
predict, dimRedResult-method
  (dimRedResult-class), 15
print, dimRedResult-method
  (dimRedResult-class), 15
Q_global, 51
Q_local, 51
Q_local (Q_local,dimRedResult-method), 53
Q_NX, 36
Q_NX (Q_NX,dimRedResult-method), 53
Q_NX (Q_NX, dimRedResult-method, 53
quality (quality,dimRedResult-method), 50
quality, dimRedResult-method, 50
quality, dimRedResult
  (quality, dimRedResult), 50
reconstruction_error
  (reconstruction_error,dimRedResult-method), 54
reconstruction_error, dimRedResult-method, 54
reconstruction_rmse, 51
reconstruction_rmse
  (reconstruction_rmse,dimRedResult-method), 55
reconstruction_rmse, dimRedResult-method, 55
Rtsne, 58
spec.emb, 36
total_correlation, 51
total_correlation
  (total_correlation, dimRedResult-method), 56
total_correlation, dimRedResult-method, 56
tSNE (tSNE-class), 57
  tSNE-class, 57

UMAP (UMAP-class), 58
  umap, 59
  UMAP-class, 58
  umap.defaults, 59