

Package ‘TDAkit’

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Type Package

Title Toolkit for Topological Data Analysis

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Description Topological data analysis studies structure and shape of the data using topological features. We provide a variety of algorithms to learn with persistent homology of the data based on functional summaries for clustering, hypothesis testing, visualization, and others. We refer to Wasserman (2018) <[doi:10.1146/annurev-statistics-031017-100045](https://doi.org/10.1146/annurev-statistics-031017-100045)> for a statistical perspective on the topic.

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diag2landscape	<i>Convert Persistence Diagram into Persistence Landscape</i>
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Description

Persistence Landscape (PL) is a functional summary of persistent homology that is constructed given a homology object.

Usage

```
diag2landscape(homology, dimension = 1, k = 0, nseq = 1000)
```

Arguments

homology	an object of S3 class "homology" generated from diagRips or other homology-generating functions.
dimension	dimension of features to be considered (default: 1).
k	the number of top landscape functions to be used (default: 0). When k=0 is set, it gives all relevant landscape functions that are non-zero.
nseq	grid size for which the landscape function is evaluated (default: 1000).

Value

a list object of "landscape" class containing

lambda an $(nseq \times k)$ landscape functions.

tseq a length-nseq vector of domain grid.

dimension dimension of features considered.

References

Peter Bubenik (2018). "The Persistence Landscape and Some of Its Properties." *arXiv:1810.04963*.

Examples

```

# -----
#           Persistence Landscape of 'iris' Dataset
#
# We will extract landscapes of dimensions 0, 1, and 2.
# For each feature, only the top 5 landscape functions are plotted.
# -----
## Prepare 'iris' data
XX = as.matrix(iris[,1:4])

## Compute Persistence Diagram
pdrips = diagRips(XX, maxdim=2)

## Convert to Landscapes of Each Dimension
land0 <- diag2landscape(pdrips, dimension=0, k=5)
land1 <- diag2landscape(pdrips, dimension=1, k=5)
land2 <- diag2landscape(pdrips, dimension=2, k=5)

## Visualize
opar <- par(no.readonly=TRUE)
par(mfrow=c(2,2))
plot(pdrips$Birth, pdrips$Death, col=as.factor(pdrips$Dimension),
     pch=19, main="persistence diagram", xlab="Birth", ylab="Death")
matplot(land0$tseq, land0$lambda, type="l", lwd=3, main="dimension 0", xlab="t")
matplot(land1$tseq, land1$lambda, type="l", lwd=3, main="dimension 1", xlab="t")
matplot(land2$tseq, land2$lambda, type="l", lwd=3, main="dimension 2", xlab="t")
par(opar)

```

diag2silhouette

Convert Persistence Diagram into Persistent Silhouette

Description

Persistence Silhouette (PS) is a functional summary of persistent homology that is constructed given a homology object. PS is a weighted average of landscape functions so that it becomes a uni-dimensional function.

Usage

```
diag2silhouette(homology, dimension = 1, p = 2, nseq = 100)
```

Arguments

homology	an object of S3 class "homology" generated from diagRips or other diagram-generating functions.
dimension	dimension of features to be considered (default: 1).
p	an exponent for the weight function of form $ a - b ^p$ (default: 2).
nseq	grid size for which the landscape function is evaluated.

Value

a list object of "silhouette" class containing

lambda an $(n_{\text{seq}} \times k)$ landscape functions.

tseq a length- n_{seq} vector of domain grid.

dimension dimension of features considered.

Examples

```
# -----
#           Persistence Silhouette of 'iris' Dataset
#
# We will extract silhouettes of dimensions 0, 1, and 2.
# -----
## Prepare 'iris' data
XX = as.matrix(iris[,1:4])

## Compute Persistence Diagram
pdrips = diagRips(XX, maxdim=2)

## Convert to Silhouettes of Each Dimension
sil0 <- diag2silhouette(pdrips, dimension=0)
sil1 <- diag2silhouette(pdrips, dimension=1)
sil2 <- diag2silhouette(pdrips, dimension=2)

## Visualize
opar <- par(no.readonly=TRUE)
par(mfrow=c(2,2))
plot(pdrips$Birth, pdrips$Death, col=as.factor(pdrips$Dimension),
     pch=19, main="persistence diagram", xlab="Birth", ylab="Death")
plot(sil0$tseq, sil0$lambda, type="l", lwd=3, main="dimension 0", xlab="t")
plot(sil1$tseq, sil1$lambda, type="l", lwd=3, main="dimension 1", xlab="t")
plot(sil2$tseq, sil2$lambda, type="l", lwd=3, main="dimension 2", xlab="t")
par(opar)
```

diagRips

Compute Vietoris-Rips Complex for Persistent Homology

Description

diagRips computes the persistent diagram of the Vietoris-Rips filtration constructed on a point cloud represented as matrix or dist object. This function is a second-hand wrapper to **TDAstats**'s wrapping for Ripser library.

Usage

```
diagRips(data, maxdim = 1, threshold = Inf)
```

Arguments

data a 'matrix' or a S3 'dist' object.
maxdim maximum dimension of the computed homological features (default: 1).
threshold maximum value of the filtration (default: Inf).

Value

a dataframe object of S3 class "homology" with following columns

Dimension dimension corresponding to a feature.

Birth birth of a feature.

Death death of a feature.

References

Raoul R. Wadhwa, Drew F.K. Williamson, Andrew Dhawan, Jacob G. Scott (2018). "TDAstats: R Pipeline for Computing Persistent Homology in Topological Data Analysis." *Journal of Open Source Software*, 3(28), 860. ISSN 2475-9066.

Ulrich Bauer (2019). "Ripsr: Efficient Computation of Vietoris-Rips Persistence Barcodes." *arXiv:1908.02518*.

See Also

[calculate_homology](#)

Examples

```

# -----
# Check consistency of two types of inputs : 'matrix' and 'dist' objects
# -----
# Use 'iris' data and compute its distance matrix
XX = as.matrix(iris[,1:4])
DX = stats::dist(XX)

# Compute VR Diagram with two inputs
vr.mat = diagRips(XX)
vr.dis = diagRips(DX)

col1 = as.factor(vr.mat$Dimension)
col2 = as.factor(vr.dis$Dimension)

# Visualize
opar <- par(no.readonly=TRUE)
par(mfrow=c(1,2), pty="s")
plot(vr.mat$Birth, vr.mat$Death, pch=19, col=col1, main="from 'matrix'")
plot(vr.dis$Birth, vr.dis$Death, pch=19, col=col2, main="from 'dist'")
par(opar)

```

fsdist

*Pairwise L_p Distance of Multiple Functional Summaries***Description**

Given multiple functional summaries $\Lambda_1(t), \Lambda_2(t), \dots, \Lambda_N(t)$, compute L_p distance in a pairwise sense.

Usage

```
fsdist(fslist, p = 2, as.dist = TRUE)
```

Arguments

fslist	a length- N list of functional summaries of persistent diagrams.
p	an exponent in $[1, \infty)$ (default: 2).
as.dist	logical; if TRUE, it returns dist object, else it returns an $(N \times N)$ symmetric matrix.

Value

a S3 dist object or $(N \times N)$ symmetric matrix of pairwise distances according to as.dist parameter.

Examples

```
# -----
#       Compute L_2 Distance for 3 Types of Landscapes and Silhouettes
#
# We will compare dim=0,1 with top-5 landscape functions with
# - Class 1 : 'iris' dataset with noise
# - Class 2 : samples from 'gen2holes()'
# - Class 3 : samples from 'gen2circles()'
# -----
## Generate Data and Diagram from VR Filtration
ndata    = 10
list_rips = list()
for (i in 1:ndata){
  dat1 = as.matrix(iris[,1:4]) + matrix(rnorm(150*4), ncol=4)
  dat2 = gen2holes(n=100, sd=1)$data
  dat3 = gen2circles(n=100, sd=1)$data

  list_rips[[i]] = diagRips(dat1, maxdim=1)
  list_rips[[i+ndata]] = diagRips(dat2, maxdim=1)
  list_rips[[i+(2*ndata)]] = diagRips(dat3, maxdim=1)
}

## Compute Persistence Landscapes from Each Diagram with k=5 Functions
```

```

# We try to get distance in dimensions 0 and 1.
list_land0 = list()
list_land1 = list()
for (i in 1:(3*ndata)){
  list_land0[[i]] = diag2landscape(list_rips[[i]], dimension=0, k=5)
  list_land1[[i]] = diag2landscape(list_rips[[i]], dimension=1, k=5)
}

## Compute Silhouettes
list_sil0 = list()
list_sil1 = list()
for (i in 1:(3*ndata)){
  list_sil0[[i]] = diag2silhouette(list_rips[[i]], dimension=0)
  list_sil1[[i]] = diag2silhouette(list_rips[[i]], dimension=1)
}

## Compute L2 Distance Matrices
ldmat0 = fsdist(list_land0, p=2, as.dist=FALSE)
ldmat1 = fsdist(list_land1, p=2, as.dist=FALSE)
sdmat0 = fsdist(list_sil0, p=2, as.dist=FALSE)
sdmat1 = fsdist(list_sil1, p=2, as.dist=FALSE)

## Visualize
opar <- par(no.readonly=TRUE)
par(mfrow=c(2,2), pty="s")
image(ldmat0[, (3*(ndata)):1], axes=FALSE, main="Landscape : dim=0")
image(ldmat1[, (3*(ndata)):1], axes=FALSE, main="Landscape : dim=1")
image(sdmat0[, (3*(ndata)):1], axes=FALSE, main="Silhouette : dim=0")
image(sdmat1[, (3*(ndata)):1], axes=FALSE, main="Silhouette : dim=1")
par(opar)

```

fsdist2

Pairwise L_p Distance for Two Sets of Functional Summaries

Description

Given two sets of functional summaries $\Lambda_1(t), \dots, \Lambda_M(t)$ and $\Omega_1(t), \dots, \Omega_N(t)$, compute L_p distance across pairs.

Usage

```
fsdist2(fslist1, fslist2, p = 2)
```

Arguments

fslist1	a length- M list of functional summaries of persistent diagrams.
fslist2	a length- N list of functional summaries of persistent diagrams.
p	an exponent in $[1, \infty)$ (default: 2).

Value

an $(M \times N)$ distance matrix.

Examples

```
# -----
#           Compute L1 and L2 Distance for Two Sets of Landscapes
#
# First set consists of {Class 1, Class 2}, while
# Second set consists of {Class 1, Class 3} where
#
# - Class 1 : 'iris' dataset with noise
# - Class 2 : samples from 'gen2holes()'
# - Class 3 : samples from 'gen2circles()'
# -----
## Generate Data and Diagram from VR Filtration
ndata      = 10
list_rips1 = list()
list_rips2 = list()
for (i in 1:ndata){
  dat1 = as.matrix(iris[,1:4]) + matrix(rnorm(150*4, sd=4), ncol=4)
  dat2 = gen2holes(n=100, sd=1)$data
  dat3 = as.matrix(iris[,1:4]) + matrix(rnorm(150*4, sd=4), ncol=4)
  dat4 = gen2circles(n=100, sd=1)$data

  list_rips1[[i]]      = diagRips(dat1, maxdim=1)
  list_rips1[[i+ndata]] = diagRips(dat2, maxdim=1)

  list_rips2[[i]]      = diagRips(dat3, maxdim=1)
  list_rips2[[i+ndata]] = diagRips(dat4, maxdim=1)
}

## Compute Persistence Landscapes from Each Diagram with k=10 Functions
# We try to get distance in dimension 1 only for faster comparison.
list_pset1 = list()
list_pset2 = list()
for (i in 1:(2*ndata)){
  list_pset1[[i]] = diag2landscape(list_rips1[[i]], dimension=1, k=10)
  list_pset2[[i]] = diag2landscape(list_rips2[[i]], dimension=1, k=10)
}

## Compute L1 and L2 Distance Matrix
dmat1 = fsdist2(list_pset1, list_pset2, p=1)
dmat2 = fsdist2(list_pset1, list_pset2, p=2)

## Visualize
opar <- par(no.readonly=TRUE)
par(mfrow=c(1,2), pty="s")
image(dmat1[(2*ndata):1], axes=FALSE, main="distance for p=1")
image(dmat2[(2*ndata):1], axes=FALSE, main="distance for p=2")
par(opar)
```


fseqdist

*Multi-sample Energy Test of Equal Distributions***Description**

Also known as k -sample problem, it tests whether multiple functional summaries are equally distributed or not via Energy statistics.

Usage

```
fseqdist(fslist, label, method = c("original", "disco"), mc.iter = 999)
```

Arguments

fslist a length- N list of functional summaries of persistent diagrams.
label a length- N vector of class labels.
method (case-sensitive) name of methods; one of "original" or "disco".
mc.iter number of bootstrap replicates.

Value

a (list) object of S3 class `htest` containing:

method name of the test.

statistic a test statistic.

p.value p -value under H_0 of equal distributions.

Examples

```
# -----
#           Test for Equality of Distributions via Energy Statistics
#
# We will compare dim=0's top-5 landscape functions with
# - Class 1 : 'iris' dataset with noise
# - Class 2 : samples from 'gen2holes()'
# - Class 3 : samples from 'gen2circles()'
# -----
## Generate Data and Diagram from VR Filtration
ndata      = 10
list_rips = list()
for (i in 1:ndata){
  dat1 = as.matrix(iris[,1:4]) + matrix(rnorm(150*4), ncol=4)
  dat2 = gen2holes(n=100, sd=1)$data
  dat3 = gen2circles(n=100, sd=1)$data
```

```

list_rips[[i]] = diagRips(dat1, maxdim=1)
list_rips[[i+ndata]] = diagRips(dat2, maxdim=1)
list_rips[[i+(2*ndata)]] = diagRips(dat3, maxdim=1)
}

## Compute Persistence Landscapes from Each Diagram with k=5 Functions
list_land0 = list()
for (i in 1:(3*ndata)){
  list_land0[[i]] = diag2landscape(list_rips[[i]], dimension=0, k=5)
}

## Create Label and Run the Test with Different Options
list_lab = c(rep(1,ndata), rep(2,ndata), rep(3,ndata))
fseqdist(list_land0, list_lab, method="original")
fseqdist(list_land0, list_lab, method="disco")

```

fshclust

Hierarchical Agglomerative Clustering

Description

Given multiple functional summaries $\Lambda_1(t), \Lambda_2(t), \dots, \Lambda_N(t)$, perform hierarchical agglomerative clustering with L_2 distance.

Usage

```

fshclust(
  fslist,
  method = c("single", "complete", "average", "mcquitty", "ward.D", "ward.D2",
    "centroid", "median"),
  members = NULL
)

```

Arguments

fslist	a length- N list of functional summaries of persistent diagrams.
method	agglomeration method to be used. This must be one of "single", "complete", "average", "mcquitty", "ward.D", "ward.D2", "centroid" or "median".
members	NULL or a vector whose length equals the number of observations. See hclust for details.

Value

an object of class `hclust`. See [hclust](#) for details.

Examples

```

# -----
#           K-Groups Clustering via Energy Distance
#
# We will cluster dim=0 under top-5 landscape functions with
# - Class 1 : 'iris' dataset with noise
# - Class 2 : samples from 'gen2holes()'
# - Class 3 : samples from 'gen2circles()'
# -----
## Generate Data and Diagram from VR Filtration
ndata      = 10
list_rips = list()
for (i in 1:ndata){
  dat1 = as.matrix(iris[,1:4]) + matrix(rnorm(150*4), ncol=4)
  dat2 = gen2holes(n=100, sd=1)$data
  dat3 = gen2circles(n=100, sd=1)$data

  list_rips[[i]] = diagRips(dat1, maxdim=1)
  list_rips[[i+ndata]] = diagRips(dat2, maxdim=1)
  list_rips[[i+(2*ndata)]] = diagRips(dat3, maxdim=1)
}
list_lab = c(rep(1,ndata), rep(2,ndata), rep(3,ndata))

## Compute Persistence Landscapes from Each Diagram with k=5 Functions
list_land0 = list()
for (i in 1:(3*ndata)){
  list_land0[[i]] = diag2landscape(list_rips[[i]], dimension=0, k=5)
}

## Run MDS for Visualization
embed = fsmds(list_land0, ndim=2)

## Clustering with 'single' and 'complete' linkage
hc.sing <- fshclust(list_land0, method="single")
hc.comp <- fshclust(list_land0, method="complete")

## Visualize
opar = par(no.readonly=TRUE)
par(mfrow=c(1,3))
plot(embed, pch=19, col=list_lab, main="2-dim embedding")
plot(hc.sing, main="single linkage")
plot(hc.comp, main="complete linkage")
par(opar)

```

Description

Given N functional summaries $\Lambda_1(t), \Lambda_2(t), \dots, \Lambda_N(t)$, perform k -groups clustering by energy distance using L_2 metric.

Usage

```
fskgroups(fslist, k = 2, ...)
```

Arguments

<code>fslist</code>	a length- N list of functional summaries of persistent diagrams.
<code>k</code>	the number of clusters.
<code>...</code>	extra parameters including
	maxiter the number of iterations (default: 50).
	nstart the number of restarts (default: 2).

Value

a length- N vector of class labels (from 1 : k).

Examples

```
# -----
#           K-Groups Clustering via Energy Distance
#
# We will cluster dim=0 under top-5 landscape functions with
# - Class 1 : 'iris' dataset with noise
# - Class 2 : samples from 'gen2holes()'
# - Class 3 : samples from 'gen2circles()'
# -----
## Generate Data and Diagram from VR Filtration
ndata = 10
list_rips = list()
for (i in 1:ndata){
  dat1 = as.matrix(iris[,1:4]) + matrix(rnorm(150*4), ncol=4)
  dat2 = gen2holes(n=100, sd=1)$data
  dat3 = gen2circles(n=100, sd=1)$data

  list_rips[[i]] = diagRips(dat1, maxdim=1)
  list_rips[[i+ndata]] = diagRips(dat2, maxdim=1)
  list_rips[[i+(2*ndata)]] = diagRips(dat3, maxdim=1)
}

## Compute Persistence Landscapes from Each Diagram with k=5 Functions
list_land0 = list()
for (i in 1:(3*ndata)){
  list_land0[[i]] = diag2landscape(list_rips[[i]], dimension=0, k=5)
}
```

```

## Run K-Groups Clustering with different K's
label2 = fskgroups(list_land0, k=2)
label3 = fskgroups(list_land0, k=3)
label4 = fskgroups(list_land0, k=4)
truelab = rep(c(1,2,3), each=ndata)

## Run MDS & Visualization
embed = fsmds(list_land0, ndim=2)
opar = par(no.readonly=TRUE)
par(mfrow=c(2,2), pty="s")
plot(embed, col=truelab, pch=19, main="true label")
plot(embed, col=label2, pch=19, main="k=2 label")
plot(embed, col=label3, pch=19, main="k=3 label")
plot(embed, col=label4, pch=19, main="k=4 label")
par(opar)

```

fskmedoids

K-Medoids Clustering

Description

Given N functional summaries $\Lambda_1(t), \Lambda_2(t), \dots, \Lambda_N(t)$, perform k-medoids clustering using pairwise distances using L_2 metric.

Usage

```
fskmedoids(fslist, k = 2)
```

Arguments

fslist a length- N list of functional summaries of persistent diagrams.
k the number of clusters.

Value

a length- N vector of class labels (from 1 : k).

Examples

```

# -----
#           K-Groups Clustering via Energy Distance
#
# We will cluster dim=0 under top-5 landscape functions with
# - Class 1 : 'iris' dataset with noise
# - Class 2 : samples from 'gen2holes()'
# - Class 3 : samples from 'gen2circles()'

```

```

# -----
## Generate Data and Diagram from VR Filtration
ndata      = 10
list_rips = list()
for (i in 1:ndata){
  dat1 = as.matrix(iris[,1:4]) + matrix(rnorm(150*4), ncol=4)
  dat2 = gen2holes(n=100, sd=1)$data
  dat3 = gen2circles(n=100, sd=1)$data

  list_rips[[i]] = diagRips(dat1, maxdim=1)
  list_rips[[i+ndata]] = diagRips(dat2, maxdim=1)
  list_rips[[i+(2*ndata)]] = diagRips(dat3, maxdim=1)
}

## Compute Persistence Landscapes from Each Diagram with k=5 Functions
list_land0 = list()
for (i in 1:(3*ndata)){
  list_land0[[i]] = diag2landscape(list_rips[[i]], dimension=0, k=5)
}

## Run K-Medoids Clustering with different K's
label2 = fskmedoids(list_land0, k=2)
label3 = fskmedoids(list_land0, k=3)
label4 = fskmedoids(list_land0, k=4)
truelab = rep(c(1,2,3), each=ndata)

## Run MDS & Visualization
embed = fsmDs(list_land0, ndim=2)
opar = par(no.readonly=TRUE)
par(mfrow=c(2,2), pty="s")
plot(embed, col=truelab, pch=19, main="true label")
plot(embed, col=label2, pch=19, main="k=2 label")
plot(embed, col=label3, pch=19, main="k=3 label")
plot(embed, col=label4, pch=19, main="k=4 label")
par(opar)

```

fsmDs

Multidimensional Scaling

Description

Given multiple functional summaries $\Lambda_1(t), \Lambda_2(t), \dots, \Lambda_N(t)$, apply multidimensional scaling to get low-dimensional representation in Euclidean space. Usually, $\text{ndim}=2, 3$ is chosen for visualization.

Usage

```
fsmDs(fslist, ndim = 2, method = c("classical", "metric"))
```

Arguments

`fslist` a length- N list of functional summaries of persistent diagrams.
`ndim` an integer-valued target dimension (default: 2).
`method` name of an algorithm type (default: classical).

Value

an $(N \times ndim)$ matrix of embedding.

Examples

```
# -----
#   Multidimensional Scaling for Multiple Landscapes and Silhouettes
#
# We will compare dim=0 with top-5 landscape and silhouette functions with
# - Class 1 : 'iris' dataset with noise
# - Class 2 : samples from 'gen2holes()'
# - Class 3 : samples from 'gen2circles()'
# -----
## Generate Data and Diagram from VR Filtration
ndata = 10
list_rips = list()
for (i in 1:ndata){
  dat1 = as.matrix(iris[,1:4]) + matrix(rnorm(150*4), ncol=4)
  dat2 = gen2holes(n=100, sd=1)$data
  dat3 = gen2circles(n=100, sd=1)$data

  list_rips[[i]] = diagRips(dat1, maxdim=1)
  list_rips[[i+ndata]] = diagRips(dat2, maxdim=1)
  list_rips[[i+(2*ndata)]] = diagRips(dat3, maxdim=1)
}

## Compute Landscape and Silhouettes of Dimension 0
list_land = list()
list_sils = list()
for (i in 1:(3*ndata)){
  list_land[[i]] = diag2landscape(list_rips[[i]], dimension=0)
  list_sils[[i]] = diag2silhouette(list_rips[[i]], dimension=0)
}
list_lab = rep(c(1,2,3), each=ndata)

## Run Classical/Metric Multidimensional Scaling
land_cmds = fsmDs(list_land, method="classical")
land_mmds = fsmDs(list_land, method="metric")
sils_cmds = fsmDs(list_sils, method="classical")
sils_mmds = fsmDs(list_sils, method="metric")

## Visualize
opar <- par(no.readonly=TRUE)
par(mfrow=c(2,2))
```

```

plot(land_cmds, pch=19, col=list_lab, main="Landscape+CMDS")
plot(land_mmds, pch=19, col=list_lab, main="Landscape+MMDS")
plot(sils_cmds, pch=19, col=list_lab, main="Silhouette+CMDS")
plot(sils_mmds, pch=19, col=list_lab, main="Silhouette+MMDS")
par(opar)

```

fsmean

Mean of Multiple Functional Summaries

Description

Given multiple functional summaries $\Lambda_1(t), \Lambda_2(t), \dots, \Lambda_N(t)$, compute the mean

$$\bar{\Lambda}(t) = \frac{1}{N} \sum_{n=1}^N \Lambda_n(t)$$

Usage

```
fsmean(fslist)
```

Arguments

`fslist` a length- N list of functional summaries of persistent diagrams.

Value

a functional summary object.

Examples

```

# -----
#           Mean of 10 Persistence Landscapes from '2holes' data
# -----
## Generate 10 Diagrams with 'gen2holes()' function
list_rips = list()
for (i in 1:10){
  list_rips[[i]] = diagRips(gen2holes(n=100, sd=2)$data, maxdim=1)
}

## Compute Persistence Landscapes from Each Diagram with k=5 Functions
list_land = list()
for (i in 1:10){
  list_land[[i]] = diag2landscape(list_rips[[i]], dimension=0, k=5)
}

## Compute Weighted Sum of Landscapes

```



```

ldsum = fsmean(list_land)

## Visualize
sam5 <- sort(sample(1:10, 5, replace=FALSE))
opar <- par(no.readonly=TRUE)
par(mfrow=c(2,3), pty="s")
for (i in 1:5){
  tgt = list_land[[sam5[i]]]
  matplot(tgt$tseq, tgt$lambda[,1:5], type="l", lwd=3, main=paste("landscape no.", sam5[i]))
}
matplot(ldsum$tseq, ldsum$lambda[,1:5], type="l", lwd=3, main="weighted sum")
par(opar)

```

fsnorm

L_p Norm of a Single Functional Summary

Description

Given a functional summary $\Lambda(t)$, compute the p -norm.

Usage

```
fsnorm(fsobj, p = 2)
```

Arguments

`fsobj` a functional summary object.
`p` an exponent in $[1, \infty)$ (default: 2).

Value

an L_p -norm value.

Examples

```

## Generate Toy Data from 'gen2circles()'
dat = gen2circles(n=100)$data

## Compute PD, Landscapes, and Silhouettes
myPD = diagRips(dat, maxdim=1)
myPL0 = diag2landscape(myPD, dimension=0)
myPL1 = diag2landscape(myPD, dimension=1)
myPS0 = diag2silhouette(myPD, dimension=0)
myPS1 = diag2silhouette(myPD, dimension=1)

## Compute 2-norm
fsnorm(myPL0, p=2)

```

```
fsnorm(myPL1, p=2)
fsnorm(myPS0, p=2)
fsnorm(myPS1, p=2)
```

fssc05Z

Spectral Clustering by Zelnik-Manor and Perona (2005)

Description

Given N functional summaries $\Lambda_1(t), \Lambda_2(t), \dots, \Lambda_N(t)$, perform spectral clustering proposed by Zelnik-Manor and Perona using a set of data-driven bandwidth parameters.

Usage

```
fssc05Z(fslist, k = 2, nnbd = 5)
```

Arguments

fslist	a length- N list of functional summaries of persistent diagrams.
k	the number of cluster (default: 2).
nnbd	neighborhood size to define data-driven bandwidth parameter (default: 5).

Value

a length- N vector of class labels (from 1 : k).

References

Zelnik-manor L, Perona P (2005). “Self-Tuning Spectral Clustering.” In Saul LK, Weiss Y, Bottou L (eds.), *Advances in Neural Information Processing Systems 17*, 1601–1608. MIT Press.

Examples

```
# -----
#           Spectral Clustering Clustering via Energy Distance
#
# We will cluster dim=0 under top-5 landscape functions with
# - Class 1 : 'iris' dataset with noise
# - Class 2 : samples from 'gen2holes()'
# - Class 3 : samples from 'gen2circles()'
# -----
## Generate Data and Diagram from VR Filtration
ndata      = 10
list_rips = list()
for (i in 1:ndata){
  dat1 = as.matrix(iris[,1:4]) + matrix(rnorm(150*4), ncol=4)
```

```

dat2 = gen2holes(n=100, sd=1)$data
dat3 = gen2circles(n=100, sd=1)$data

list_rips[[i]] = diagRips(dat1, maxdim=1)
list_rips[[i+ndata]] = diagRips(dat2, maxdim=1)
list_rips[[i+(2*ndata)]] = diagRips(dat3, maxdim=1)
}

## Compute Persistence Landscapes from Each Diagram with k=5 Functions
list_land0 = list()
for (i in 1:(3*ndata)){
  list_land0[[i]] = diag2landscape(list_rips[[i]], dimension=0, k=5)
}

## Run Spectral Clustering using Different K's.
label2 = fssc05Z(list_land0, k=2)
label3 = fssc05Z(list_land0, k=3)
label4 = fssc05Z(list_land0, k=4)
truelab = rep(c(1,2,3), each=ndata)

## Run MDS & Visualization
embed = fsmds(list_land0, ndim=2)
opar = par(no.readonly=TRUE)
par(mfrow=c(2,2), pty="s")
plot(embed, col=truelab, pch=19, main="true label")
plot(embed, col=label2, pch=19, main="k=2 label")
plot(embed, col=label3, pch=19, main="k=3 label")
plot(embed, col=label4, pch=19, main="k=4 label")
par(opar)

```

fssum

Weighted Sum of Multiple Functional Summaries

Description

Given multiple functional summaries $\Lambda_1(t), \Lambda_2(t), \dots, \Lambda_N(t)$, compute the weighted sum

$$\bar{\Lambda}(t) = \sum_{n=1}^N w_n \Lambda_n(t)$$

with a specified vector of given weights w_1, w_2, \dots, w_N .

Usage

```
fssum(fslist, weight = NULL)
```

Arguments

`fslist` a length- N list of functional summaries of persistent diagrams.

`weight` a weight vector of length N . If NULL (default), weights are automatically set as $w_1 = \dots = w_N = 1/N$.

Value

a functional summary object.

Examples

```
# -----
#   Weighted Average of 10 Persistence Landscapes from '2holes' data
# -----
## Generate 10 Diagrams with 'gen2holes()' function
list_rips = list()
for (i in 1:10){
  list_rips[[i]] = diagRips(gen2holes(n=100, sd=2)$data, maxdim=1)
}

## Compute Persistence Landscapes from Each Diagram with k=5 Functions
list_land = list()
for (i in 1:10){
  list_land[[i]] = diag2landscape(list_rips[[i]], dimension=0, k=5)
}

## Some Random Weights
wrand = abs(stats::rnorm(10))
wrand = wrand/sum(wrand)

## Compute Weighted Sum of Landscapes
ldsum = fssum(list_land, weight=wrand)

## Visualize
sam5 <- sort(sample(1:10, 5, replace=FALSE))
opar <- par(no.readonly=TRUE)
par(mfrow=c(2,3), pty="s")
for (i in 1:5){
  tgt = list_land[[sam5[i]]]
  matplot(tgt$tseq, tgt$lambda[,1:5], type="l", lwd=3, main=paste("landscape no.",sam5[i]))
}
matplot(ldsum$tseq, ldsum$lambda[,1:5], type="l", lwd=3, main="weighted sum")
par(opar)
```

Description

Given N functional summaries $\Lambda_1(t), \Lambda_2(t), \dots, \Lambda_N(t)$, t-SNE mimicks the pattern of probability distributions over pairs of Banach-valued objects on low-dimensional target embedding space by minimizing Kullback-Leibler divergence.

Usage

```
fstsne(fslist, ndim = 2, ...)
```

Arguments

fslist a length- N list of functional summaries of persistent diagrams.
ndim an integer-valued target dimension.
... extra parameters for [Rtsne](#) algorithm, such as perplexity, momentum, and others.

Value

a named list containing

embed an $(N \times ndim)$ matrix whose rows are embedded observations.

stress discrepancy between embedded and original distances as a measure of error.

See Also

[Rtsne](#)

Examples

```
# -----
#   Multidimensional Scaling for Multiple Landscapes and Silhouettes
#
# We will compare dim=0 with top-5 landscape and silhouette functions with
# - Class 1 : 'iris' dataset with noise
# - Class 2 : samples from 'gen2holes()'
# - Class 3 : samples from 'gen2circles()'
# -----
## Generate Data and Diagram from VR Filtration
ndata    = 10
list_rips = list()
for (i in 1:ndata){
  dat1 = as.matrix(iris[,1:4]) + matrix(rnorm(150*4), ncol=4)
  dat2 = gen2holes(n=100, sd=1)$data
  dat3 = gen2circles(n=100, sd=1)$data

  list_rips[[i]] = diagRips(dat1, maxdim=1)
  list_rips[[i+ndata]] = diagRips(dat2, maxdim=1)
  list_rips[[i+(2*ndata)]] = diagRips(dat3, maxdim=1)
}
```

```

## Compute Landscape and Silhouettes of Dimension 0
list_land = list()
list_sils = list()
for (i in 1:(3*ndata)){
  list_land[[i]] = diag2landscape(list_rips[[i]], dimension=0)
  list_sils[[i]] = diag2silhouette(list_rips[[i]], dimension=0)
}
list_lab = rep(c(1,2,3), each=ndata)

## Run t-SNE and Classical/Metric MDS
land_cmds = fsmds(list_land, method="classical")
land_mmds = fsmds(list_land, method="metric")
land_tsne = fstsne(list_land, perplexity=5)$embed
sils_cmds = fsmds(list_sils, method="classical")
sils_mmds = fsmds(list_sils, method="metric")
sils_tsne = fstsne(list_land, perplexity=5)$embed

## Visualize
opar <- par(no.readonly=TRUE)
par(mfrow=c(2,3))
plot(land_cmds, pch=19, col=list_lab, main="Landscape+CMDS")
plot(land_mmds, pch=19, col=list_lab, main="Landscape+MMDS")
plot(land_tsne, pch=19, col=list_lab, main="Landscape+tSNE")
plot(sils_cmds, pch=19, col=list_lab, main="Silhouette+CMDS")
plot(sils_mmds, pch=19, col=list_lab, main="Silhouette+MMDS")
plot(sils_tsne, pch=19, col=list_lab, main="Silhouette+tSNE")
par(opar)

```

gen2circles

Generate Two Intersecting Circles

Description

It generates data from two intersecting circles.

Usage

```
gen2circles(n = 496, sd = 0)
```

Arguments

n	the total number of observations to be generated.
sd	level of additive white noise.

Value

a list containing

data an $(n \times 2)$ data matrix for row-stacked observations.

label a length- n vector for class label.

Examples

```
## Generate Data with Different Noise Levels
nn = 200
x1 = gen2circles(n=nn, sd=0)
x2 = gen2circles(n=nn, sd=0.1)
x3 = gen2circles(n=nn, sd=0.25)

## Visualize
opar <- par(no.readonly=TRUE)
par(mfrow=c(1,3), pty="s")
plot(x1$data, pch=19, main="sd=0.00", col=x1$label)
plot(x2$data, pch=19, main="sd=0.10", col=x2$label)
plot(x3$data, pch=19, main="sd=0.25", col=x3$label)
par(opar)
```

gen2holes

Generate Two Intertwined Holes

Description

It generates data from two intertwine circles with empty interiors(holes).

Usage

```
gen2holes(n = 496, sd = 0)
```

Arguments

n the total number of observations to be generated.

sd level of additive white noise.

Value

a list containing

data an $(n \times 2)$ data matrix for row-stacked observations.

label a length- n vector for class label.

Examples

```
## Generate Data with Different Noise Levels
nn = 200
x1 = gen2holes(n=nn, sd=0)
x2 = gen2holes(n=nn, sd=0.1)
x3 = gen2holes(n=nn, sd=0.25)

## Visualize
opar <- par(no.readonly=TRUE)
par(mfrow=c(1,3), pty="s")
plot(x1$data, pch=19, main="sd=0.00", col=x1$label)
plot(x2$data, pch=19, main="sd=0.10", col=x2$label)
plot(x3$data, pch=19, main="sd=0.25", col=x3$label)
par(opar)
```

plkernel

Persistence Landscape Kernel

Description

Given multiple persistence landscapes $\Lambda_1(t), \Lambda_2(t), \dots, \Lambda_N(t)$, compute the persistence landscape kernel under the L_2 sense.

Usage

```
plkernel(landlist)
```

Arguments

landlist a length- N list of "landscape" objects, which can be obtained from [diag2landscape](#) function.

Value

an $(N \times N)$ kernel matrix.

References

Jan Reininghaus, Stefan Huber, Ulrich Bauer, and Roland Kwitt (2015). "A stable multi-scale kernel for topological machine learning." *Proc. 2015 IEEE Conf. Comp. Vision & Pat. Rec. (CVPR '15)*.

Examples

```
# -----
# Persistence Landscape Kernel in Dimension 0 and 1
#
# We will compare dim=0,1 with top-20 landscape functions with
```



```

# - Class 1 : 'iris' dataset with noise
# - Class 2 : samples from 'gen2holes()'
# - Class 3 : samples from 'gen2circles()'
# -----
## Generate Data and Diagram from VR Filtration
ndata      = 10
list_rips = list()
for (i in 1:ndata){
  dat1 = as.matrix(iris[,1:4]) + matrix(rnorm(150*4), ncol=4)
  dat2 = gen2holes(n=100, sd=1)$data
  dat3 = gen2circles(n=100, sd=1)$data

  list_rips[[i]] = diagRips(dat1, maxdim=1)
  list_rips[[i+ndata]] = diagRips(dat2, maxdim=1)
  list_rips[[i+(2*ndata)]] = diagRips(dat3, maxdim=1)
}

## Compute Persistence Landscapes from Each Diagram with k=5 Functions
# We try to get distance in dimensions 0 and 1.
list_land0 = list()
list_land1 = list()
for (i in 1:(3*ndata)){
  list_land0[[i]] = diag2landscape(list_rips[[i]], dimension=0, k=5)
  list_land1[[i]] = diag2landscape(list_rips[[i]], dimension=1, k=5)
}

## Compute Persistence Landscape Kernel Matrix
plk0 <- plkernel(list_land0)
plk1 <- plkernel(list_land1)

## Visualize
opar <- par(no.readonly=TRUE)
par(mfrow=c(1,2), pty="s")
image(plk0[, (3*(ndata)):1], axes=FALSE, main="Kernel : dim=0")
image(plk1[, (3*(ndata)):1], axes=FALSE, main="Kernel : dim=1")
par(opar)

```

plot.homology

Plot Persistent Homology via Barcode or Diagram

Description

Given a persistent homology of the data represented by a reconstructed complex in S3 class homology object, visualize it as either a barcode or a persistence diagram using **ggplot2**.

Usage

```

## S3 method for class 'homology'
plot(x, ...)

```

Arguments

`x` a homology object.
`...` extra parameters including **method** type of visualization; either "barcode" or "diagram".

Value

a **ggplot2** object.

Examples

```
# Use 'iris' data
XX = as.matrix(iris[,1:4])

# Compute VR Diagram
homology = diagRips(XX)

# Plot with 'barcode'
opar <- par(no.readonly=TRUE)
plot(homology, method="barcode")
par(opar)
```

plot.landscape

Plot Persistence Landscape

Description

Given a persistence landscape object in S3 class `landscape`, visualize the landscapes using **ggplot2**.

Usage

```
## S3 method for class 'landscape'
plot(x, ...)
```

Arguments

`x` a landscape object.
`...` extra parameters including **top.k** the number of landscapes to be plotted (default: 5).
colored a logical; TRUE to assign different colors for landscapes, or FALSE to use grey color for all landscapes.

Value

a **ggplot2** object.

Examples

```
# Use 'iris' data
XX = as.matrix(iris[,1:4])

# Compute Persistence diagram and landscape of order 0
homology = diagRips(XX)
landscape = diag2landscape(homology, dimension=0)

# Plot with 'barcode'
opar <- par(no.readonly=TRUE)
plot(landscape)
par(opar)
```

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