## Package 'phutil'

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Title Persistence Homology Utilities

Version 0.0.1

Description A low-level package for hosting persistence data. It is part of the 'TDAverse' suite of packages, which is designed to provide a collection of packages for enabling machine learning and data science tasks using persistent homology. Implements a class for hosting persistence data, a number of coercers from and to already existing and used data structures from other packages and functions to compute distances between persistence diagrams. A formal definition and study of bottleneck and Wasserstein distances can be found in Bubenik, Scott and Stanley (2023)
 <doi:10.1007/s41468-022-00103-8>. Their implementation in 'phutil' relies on the 'C++' Hera library developed by Kerber, Morozov and Nigmetov (2017)
 <doi:10.1145/3064175>.

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URL https://github.com/tdaverse/phutil,

https://tdaverse.github.io/phutil/

BugReports https://github.com/tdaverse/phutil/issues

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arch\_spirals

A sample of persistence diagrams from the arch spiral

## Description

A collection of 24 samples of size 120 on the arch spiral from which a persistence diagram is computed using the TDA::ripsDiag() function with maxdimension = 2 and maxscale = 6. Each diagram has been generated using the tdaunif::sample\_arch\_spiral() function with the following parameters: n = 120, arms = 2<sup>\*\*</sup> and sd = 0.05<sup>\*</sup>. The seed was fixed to 28415.

## Usage

```
arch_spirals
```

#### Format

A list of length 24, where each element is an object of class 'persistence'.

distances

#### Description

This collection of functions computes the distance between two persistence diagrams of the same homology dimension. The diagrams must be represented as 2-column matrices. The first column of the matrix contains the birth times and the second column contains the death times of the points.

## Usage

```
bottleneck_distance(
  х,
 у,
  tol = sqrt(.Machine$double.eps),
  validate = TRUE,
  dimension = 0L
)
wasserstein_distance(
  х,
 у,
  tol = sqrt(.Machine$double.eps),
  p = 1,
  validate = TRUE,
  dimension = 0L
)
kantorovich_distance(
  х,
 у,
  tol = sqrt(.Machine$double.eps),
  p = 1,
  validate = TRUE,
  dimension = 0L
)
```

## Arguments

x	Either a matrix of shape $n \times 2$ or an object of class persistence specifying the first persistence diagram.
У	Either a matrix of shape $m \times 2$ or an object of class persistence specifying the second persistence diagram.
tol	A numeric value specifying the relative error. Defaults to $sqrt(.Machine$double.eps)$ For the Bottleneck distance, it can be set to 0.0 in which case the exact Bottle- neck distance is computed, while an approximate Bottleneck distance is com- puted if tol > 0.0. For the Wasserstein distance, it must be strictly positive.

validate	A boolean value specifying whether to validate the input persistence diagrams. Defaults to TRUE. If FALSE, the function will not check if the input persistence diagrams are valid. This can be useful for performance reasons, but it is recom- mended to keep it TRUE for safety.
dimension	An integer value specifying the homology dimension for which to compute the distance. Defaults to $0L$ . This is only used if x and y are objects of class persistence.
р	A numeric value specifying the power for the Wasserstein distance. Defaults to $1.0$ .

## Details

A matching  $\varphi : D_1 \to D_2$  between persistence diagrams is a bijection of multisets, where both diagrams are assumed to have all points on the diagonal with infinite multiplicity. The *p*-Wasserstein distance between  $D_1$  and  $D_2$  is defined as the infimum over all matchings of the expression

$$W_p(D_1, D_2) = \inf_{\varphi: D_1 \to D_2} \left( \sum_{x \in D_1} \|x - \varphi(x)\|^p \right)^{\frac{1}{p}}$$

that can be thought of as the Minkowski distance between the diagrams viewed as vectors on the shared coordinates defined by the matching  $\varphi$ . The norm  $\|\cdot\|$  can be arbitrary; as implemented here, it is the infinity norm  $\|(x_1, x_2)\|_{\infty} = \max(x_1, x_2)$ . In the limit  $p \to \infty$ , the Wasserstein distance becomes the *bottleneck distance*:

$$B(D_1, D_2) = \inf_{\varphi: D_1 \to D_2} \sup_{x \in D_1} \|x - \varphi(x)\|.$$

The Wasserstein metric is also called the Kantorovich metric in recognition of the originator of the metric.

#### Value

A numeric value storing either the Bottleneck or the Wasserstein distance between the two persistence diagrams.

#### See Also

the Hera C++ library

#### Examples

```
bottleneck_distance(
   persistence_sample[[1]]$pairs[[1]],
   persistence_sample[[2]]$pairs[[1]]
)
bottleneck_distance(
   persistence_sample[[1]],
   persistence_sample[[2]]
```

noisy\_circle

```
)
wasserstein_distance(
   persistence_sample[[1]]$pairs[[1]],
   persistence_sample[[2]]$pairs[[1]]
)
wasserstein_distance(
   persistence_sample[[1]],
   persistence_sample[[2]]
)
```

noisy\_circle Toy Data: Noisy circle

## Description

A simulated data set consisting of 100 points sampled from a circle with additive Gaussian noise using a standard deviation of 0.05.

#### Usage

```
noisy_circle_points
```

noisy\_circle\_ripserr

noisy\_circle\_tda\_rips

## Format

noisy\_circle\_points: A matrix with 100 rows and 2 columns listing the coordinates of the points.

#### noisy\_circle\_ripserr:

An object of class 'PHom' as returned by the **ripserr::vietoris\_rips()** function, which is a data frame with 3 variables:

- dimension: the dimension/degree of the feature,
- birth: the birth value of the feature,
- death: the death value of the feature.

#### noisy\_circle\_tda\_rips:

A list of length 1 containing an object of class 'diagram' as returned by the TDA::ripsDiag()\$diagram function, which is a matrix with 3 columns:

- dimension: the dimension/degree of the feature,
- birth: the birth value of the feature,
- death: the death value of the feature.

An object of class PHom (inherits from data.frame) with 101 rows and 3 columns.

An object of class list of length 1.

#### Details

The point cloud stored in noisy\_circle\_points has been generated using the tdaunif package using the tdaunif::sample\_circle() function. Specifically, the following parameters were used: n = 100, sd = 0.05 and a seed of 1234.

The persistence diagram stored in noisy\_circle\_ripserr has been computed using the **ripserr** package with the **ripserr::vietoris\_rips()** function. Specifically, the following parameters were used: max\_dim = 1L.

The persistence diagram stored in noisy\_circle\_tda\_rips has been computed using the **TDA** package with the **TDA::ripsDiag()** function. Specifically, the following parameters were used: maxdimension = 1L and maxscale = 1.6322.

## Source

```
https://tdaverse.github.io/tdaunif/reference/circles.html, https://tdaverse.github.
io/ripserr/reference/vietoris_rips.html, https://www.rdocumentation.org/packages/
TDA/versions/1.9.1/topics/ripsDiag
```

pairwise-distances Pairwise distances within a set of persistence diagrams

## Description

This collection of functions computes the pairwise distance matrix between all pairs in a set of persistence diagrams of the same homology dimension. The diagrams must be represented as 2-column matrices. The first column of the matrix contains the birth times and the second column contains the death times of the points.

#### Usage

```
bottleneck_pairwise_distances(
    x,
    tol = sqrt(.Machine$double.eps),
    validate = TRUE,
    dimension = 0L,
    ncores = 1L
)
wasserstein_pairwise_distances(
    x,
    tol = sqrt(.Machine$double.eps),
    p = 1,
    validate = TRUE,
    dimension = 0L,
    ncores = 1L
)
```

```
kantorovich_pairwise_distances(
    x,
    tol = sqrt(.Machine$double.eps),
    p = 1,
    validate = TRUE,
    dimension = 0L,
    ncores = 1L
)
```

## Arguments

x	A list of either 2-column matrices or objects of class persistence specifying the set of persistence diagrams.
tol	A numeric value specifying the relative error. Defaults to $sqrt(.Machine$double.eps)$ . For the Bottleneck distance, it can be set to 0.0 in which case the exact Bottle- neck distance is computed, while an approximate Bottleneck distance is com- puted if tol > 0.0. For the Wasserstein distance, it must be strictly positive.
validate	A boolean value specifying whether to validate the input persistence diagrams. Defaults to TRUE. If FALSE, the function will not check if the input persistence diagrams are valid. This can be useful for performance reasons, but it is recom- mended to keep it TRUE for safety.
dimension	An integer value specifying the homology dimension for which to compute the distance. Defaults to $0L$ . This is only used if x and y are objects of class persistence.
ncores	An integer value specifying the number of cores to use for parallel computation. Defaults to 1L.
р	A numeric value specifying the power for the Wasserstein distance. Defaults to 1.0.

## Value

An object of class 'dist' containing the pairwise distance matrix between the persistence diagrams.

## Examples

```
spl <- persistence_sample[1:10]
# Extract the list of 2-column matrices for dimension 0 in the sample
x <- lapply(spl[1:10], function(x) x$pairs[[1]])
# Compute the pairwise Bottleneck distances
Db <- bottleneck_pairwise_distances(spl)
Db <- bottleneck_pairwise_distances(x)
# Compute the pairwise Wasserstein distances
Dw <- wasserstein_pairwise_distances(spl)
Dw <- wasserstein_pairwise_distances(x)</pre>
```

```
persistence
```

#### Description

A collection of functions to coerce persistence data into objects of class persistence (See Value section for more details on this class). It is currently possible to coerce persistence data from the following sources:

- a matrix with at least 3 columns (dimension/degree, start/birth, end/death) as returned by ripserr::vietoris\_rips() in the form of the 'PHom' class,
- a list as returned by any \*Diag() function in the TDA package.

#### Usage

```
as_persistence(x, warn = TRUE, ...)
## S3 method for class 'list'
as_persistence(x, warn = TRUE, ...)
## S3 method for class 'persistence'
as_persistence(x, warn = TRUE, ...)
## S3 method for class 'data.frame'
as_persistence(x, warn = TRUE, ...)
## S3 method for class 'matrix'
as_persistence(x, warn = TRUE, ...)
## S3 method for class 'diagram'
as_persistence(x, warn = TRUE, ...)
## S3 method for class 'PHom'
as_persistence(x, ...)
## S3 method for class 'hclust'
as_persistence(x, warn = TRUE, birth = NULL, ...)
## S3 method for class 'persistence'
print(x, ...)
## S3 method for class 'persistence'
format(x, ...)
get_pairs(x, dimension, ...)
## S3 method for class 'persistence'
```

## persistence

```
as.matrix(x, ...)
## S3 method for class 'persistence'
as.data.frame(x, row.names = NULL, optional = TRUE, ...)
```

## Arguments

Suments	
x	An R object containing the persistence data to be coerced into an object of class persistence. Currently supported forms are:
	• a ≥ 2-column matrix (or object coercible to one) with dimension/degree, start/birth and end/death columns; if it has only 2 columns, we assume that the dimension column is missing and we set it to 0 (i.e. we assume that the data is in the form birth and death),
	• a base::data.frame (or object coercible to one) with at least 3 columns containing the persistence data; if it has only 2 columns, we assume that the dimension column is missing and we set it to 0,
	• a list of 2-column matrices (or objects coercible to one) with the first column being the birth and the second column being the death of homological features; indexed by dimension, i.e. the <i>i</i> -th element of the list corresponds to the $(i - 1)$ -th homology dimension,
	<ul> <li>an object of class 'PHom' as returned by ripserr::vietoris_rips(),</li> </ul>
	• (a list as returned by a *Diag() function in <b>TDA</b> (e.g. <b>TDA</b> ::ripsDiag()) whose first element is) an object of class 'diagram',
	• an object of class stats::hclust in which case we use the entry height as the death of homological features and 0 as the birth of all features.
warn	A boolean specifying whether to issue a warning if the input persistence data contained unordered pairs. Defaults to TRUE.
	Parameters passed to methods.
birth	A numeric value specifying the height at which to declare all leaves were born. Defaults to 0 if all heights are non-negative and -Inf otherwise.
dimension	A non-negative integer specifying the homology dimension for which to recover a matrix of persistence pairs.
row.names	NULL or a character vector giving the row names for the data frame. Missing values are not allowed.
optional	logical. If TRUE, setting row names and converting column names (to syntac- tic names: see make.names) is optional. Note that all of R's <b>base</b> package as.data.frame() methods use optional only for column names treatment, ba- sically with the meaning of data.frame(*, check.names = !optional). See also the make.names argument of the matrix method.

## Details

**Caution.** When providing an *unnamed* input matrix, the matrix coercer assumes that it has at least 3 columns, with the first column being the dimension/degree, the second column being the start/birth and the third column being the end/death.

## Value

An object of class persistence which is a list of 2 elements:

- pairs: A list of 2-column matrices containing birth-death pairs. The *i*-th element of the list corresponds to the (i 1)-th homology dimension. If there is no pairs for a given dimension but there are pairs in higher dimensions, the corresponding element(s) is/are filled with a  $0 \times 2$  numeric matrix.
- metadata: A list of length 6 containing information about how the data was computed:
  - orderered\_pairs: A boolean indicating whether the pairs in the pairs list are ordered (i.e. the first column is strictly less than the second column).
  - data: The name of the object containing the original data on which the persistence data was computed.
  - engine: The name of the package and the function of this package that computed the persistence data in the form "package\_name::package\_function".
  - filtration: The filtration used in the computation in a human-readable format (i.e. full names, capitals where need, etc.).
  - parameters: A list of parameters used in the computation.
  - call: The exact call that generated the persistence data.

#### Examples

```
as_persistence(noisy_circle_ripserr)
x <- as_persistence(noisy_circle_tda_rips)
x
as_persistence(x)
get_pairs(x, dimension = 1)
as.data.frame(x)
# distances between cities
euroclust <- hclust(eurodist, method = "ward.D")
as_persistence(euroclust)
# `hclust()` can accommodate negative distances
d <- as.dist(rbind(c(0, 3, -4), c(3, 0, 5), c(-4, 5, 0)))
hc <- hclust(d, method = "single")
ph <- as_persistence(hc, birth = -10)
get_pairs(ph, 0)</pre>
```

persistence-set An 'S3' class object for storing sets of persistence diagrams

#### Description

An 'S3' class object for storing sets of persistence diagrams

#### persistence\_sample

#### Usage

```
as_persistence_set(x)
## S3 method for class 'persistence_set'
format(x, ...)
## S3 method for class 'persistence_set'
print(x, ...)
```

#### Arguments

х	A list of objects of class persistence.
	Additional arguments passed to the function.

#### Value

An object of class 'persistence\_set' containing the set of persistence diagrams.

#### Examples

```
# Create a persistence set from a list of persistence diagrams
as_persistence_set(persistence_sample[1:10])
```

persistence\_sample Toy Data: A sample of persistence diagrams

## Description

A collection of 100 samples of size 100 on the sphere from which a persistence diagram is computed using the TDA::ripsDiag() function with parameters maxdimension = 1L and maxscale = 1.6322. Each diagram has been generated using the tdaunif::sample\_2sphere() function with the following parameters: n = 100 and sd = 0.05. The seed was fixed to 1234.

#### Usage

```
persistence_sample
```

#### Format

A list of length 100, where each element is an object of class 'persistence'.

trefoils

## Description

A collection of 24 samples of size 120 on the trefoil from which a persistence diagram is computed using the TDA::ripsDiag() function with maxdimension = 2 and maxscale = 6. Each diagram has been generated using the tdaunif::sample\_trefoil() function with the following parameters: n = 120 and sd = 0.05. The seed was fixed to 28415.

## Usage

trefoils

## Format

A list of length 24, where each element is an object of class 'persistence'.

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