

Package: tdarec (via r-universe)

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Title A 'recipes' Extension for Persistent Homology and Its Vectorizations

Version 0.2.1

Description Topological data analytic methods in machine learning rely on vectorizations of the persistence diagrams that encode persistent homology, as surveyed by Ali & al (2000) <[doi:10.48550/arXiv.2212.09703](https://doi.org/10.48550/arXiv.2212.09703)>. Persistent homology can be computed using 'TDA' and 'ripserr' and vectorized using 'TDAvec'. The Tidymodels package collection modularizes machine learning in R for straightforward extensibility; see Kuhn & Silge (2022, ISBN:978-1-4920-9644-3). These 'recipe' steps and 'dials' tuners make efficient algorithms for computing and vectorizing persistence diagrams available for Tidymodels workflows.

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URL <https://github.com/tdaverse/tdarec>

BugReports <https://github.com/tdaverse/tdarec/issues>

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Contents

blur	2
blur_sigmas	4
get_blur_range	5
mnist	6
step_blur	7
step_pd_degree	8
step_pd_point_cloud	10
step_pd_raster	12
step_vpd_algebraic_functions	14
step_vpd_betti_curve	17
step_vpd_complex_polynomial	19
step_vpd_descriptive_statistics	21
step_vpd_euler_characteristic_curve	24
step_vpd_normalized_life_curve	26
step_vpd_persistence_block	28
step_vpd_persistence_image	31
step_vpd_persistence_landscape	34
step_vpd_persistence_silhouette	37
step_vpd_persistent_entropy_summary	39
step_vpd_tent_template_functions	42
step_vpd_tropical_coordinates	44
vpd-dials	46
vpd-finalizers	49
vpd-summarizers	50
Index	55

blur	<i>Gaussian blur of an array</i>
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Description

This function takes a numeric array of any dimension as input and returns a blurred array of the same dimensions as output.

Usage

```
blur(
  x,
  xmin = 0,
  xmax = 2^ceiling(log(max(x + 1), 2)) - 1,
  sigma = max(dim(x))/2^(length(dim(x)) + 1)
)
```

Arguments

<code>x</code>	a numerical 'array' (including 'matrix')
<code>xmin</code>	the smallest possible value in <code>x</code> ; defaults to 0
<code>xmax</code>	the largest possible value in <code>x</code> ; defaults to the smallest integer $2^k - 1 \leq \max(x)$
<code>sigma</code>	the standard deviation of the gaussian distribution with which to convolve <code>x</code> ; defaults to $\max(\dim(x))/2^{D+1}$, where D is the dimensionality of <code>x</code>

Details

This function is adapted from `spatstat.explore::blur()`, part of the [spatstat package collection](#).

The procedure takes the following steps:

1. Rescale the value range from $[xmin, xmax]$ to $[0, 1]$.
2. Convolve `x` with $N(0, \sigma^2)$.
3. Rescale the result back to the original value range.

Value

An array of the same dimensions as `x`.

Examples

```
square <- matrix(byrow = TRUE, nrow = 6L, c(
  0, 0, 0, 0, 0, 0, 0, 0,
  0, 1, 1, 1, 1, 0, 0, 0,
  0, 1, 0, 0, 1, 1, 1, 0,
  0, 1, 0, 0, 1, 0, 1, 0,
  0, 1, 1, 1, 1, 1, 1, 0,
  0, 0, 0, 0, 0, 0, 0, 0
))
square_blur <- blur(square)
image(t(square))
image(t(square_blur))
```

 blur_sigmas

Standard deviation of Gaussian blur

Description

The standard deviation of the noise function convolved with array values to induce blur in raster data.

Usage

```
blur_sigmas(range = c(unknown(), unknown()), trans = transform_log1p())
```

Arguments

range	A two-element vector holding the <i>defaults</i> for the smallest and largest possible values, respectively. If a transformation is specified, these values should be in the <i>transformed units</i> .
trans	A trans object from the scales package, such as <code>scales::transform_log10()</code> or <code>scales::transform_reciprocal()</code> . If not provided, the default is used which matches the units used in range. If no transformation, NULL.

Details

The gaussian blur step deploys `blur()`. See there for definitions and references.

`get_blur_range()` varies the parameter logarithmically from 0 to an order of magnitude greater than the `blur()` default.

Value

A param object or list of param objects.

Examples

```
img_dat <- data.frame(img = I(list(volcano)))

(blur_man <- blur_sigmas(range = c(0, 3)))
grid_regular(blur_man)

(blur_fin <- blur_sigmas() %>% get_blur_range(x = img_dat))
grid_regular(blur_fin)
```

get_blur_range (Maximum) topological dimension or homological degree

Description

The degree of the homology group to vectorize, or the degree at which to stop vectorizing.

Usage

```
get_blur_range(object, x, ...)
```

```
hom_degree(range = c(0L, unknown()), trans = NULL)
```

```
max_hom_degree(range = c(0L, unknown()), trans = NULL)
```

```
get_hom_range(object, x, max_dim = 2L, ...)
```

Arguments

object	A param object or a list of param objects.
x	The predictor data. In some cases (see below) this should only include numeric data.
...	Other arguments to pass to the underlying parameter finalizer functions. For example, for <code>get_rbf_range()</code> , the dots are passed along to <code>kernlab::sigest()</code> .
range	A two-element vector holding the <i>defaults</i> for the smallest and largest possible values, respectively. If a transformation is specified, these values should be in the <i>transformed units</i> .
trans	A trans object from the scales package, such as <code>scales::transform_log10()</code> or <code>scales::transform_reciprocal()</code> . If not provided, the default is used which matches the units used in range. If no transformation, NULL.
max_dim	Bound on the maximum dimension determined from the data.

Details

Topological features have whole number dimensions that determine the degrees of homology that encode them. Any finite point cloud will have finite topological dimension, but most practical applications exploit features of degree at most 3.

Steps may vectorize features of a single degree (`hom_degree()`) or of degrees zero through some maximum (`max_hom_degree()`).

In case the (maximum) degree is not provided, `get_hom_range()` queries each list-column for the maximum dimension of its point cloud and returns the smaller of this maximum and `max_dim` (which defaults to 2L, the highest homological degree of interest in most practical applications).

Value

A param object or list of param objects.

Examples

```

# toy data set
klein_sampler <- function(n, prob = .5) {
  if (rbinom(1, 1, prob) == 0) {
    tdaunif::sample_klein_flat(n)
  } else {
    tdaunif::sample_klein_tube(n)
  }
}
sample_data <- data.frame(
  id = LETTERS[seq(4L)],
  sample = I(c(replicate(4L, klein_sampler(60), simplify = FALSE)))
)

# options to calibrate homological degree
hom_degree(range = c(2, 5))
hom_degree() %>% get_hom_range(x = sample_data[, 2, drop = FALSE])
hom_degree() %>% get_hom_range(x = sample_data[, 2, drop = FALSE], max_dim = 5)

# heterogeneous data types
hetero_data <- tibble(dataset = list(mtcars, nhtemp, eurodist, HairEyeColor))
hetero_data %>%
  mutate(class = vapply(dataset, function(x) class(x)[[1L]], ""))
get_hom_range(
  hom_degree(),
  hetero_data,
  max_dim = 60
)

```

mnist

MNIST handwritten digits

Description

This is a 1% stratified random sample from the MNIST handwritten digit data set.

Usage

```
mnist_train; mnist_test
```

Format

Two data frames of 600 and 100 rows, respectively, and 2 variables:

digit list column of 28×28 numeric matrices

label integer digit

Source

<http://yann.lecun.com/exdb/mnist/>

step_blur

*Blur raster data***Description**

The function `step_blur()` creates a *specification* of a recipe step that will induce Gaussian blur in numerical arrays. The input and output must be list-columns.

Usage

```
step_blur(
  recipe,
  ...,
  role = NA_character_,
  trained = FALSE,
  xmin = 0,
  xmax = 1,
  blur_sigmas = NULL,
  skip = FALSE,
  id = rand_id("blur")
)
```

Arguments

<code>recipe</code>	A recipe object. The step will be added to the sequence of operations for this recipe.
<code>...</code>	One or more selector functions to choose variables for this step. See selections() for more details.
<code>role</code>	For model terms created by this step, what analysis role should they be assigned? By default, the new columns created by this step from the original variables will be used as <i>predictors</i> in a model.
<code>trained</code>	A logical to indicate if the quantities for preprocessing have been estimated.
<code>xmin, xmax, blur_sigmas</code>	Parameters passed to blur() .
<code>skip</code>	A logical. Should the step be skipped when the recipe is baked by bake() ? While all operations are baked when prep() is run, some operations may not be able to be conducted on new data (e.g. processing the outcome variable(s)). Care should be taken when using <code>skip = TRUE</code> as it may affect the computations for subsequent operations.
<code>id</code>	A character string that is unique to this step to identify it.

Details

The gaussian blur step deploys [blur\(\)](#). See there for definitions and references.

TODO: Explain the importance of blur for PH of image data.

Value

An updated version of recipe with the new step added to the sequence of any existing operations.

Tuning Parameters

This step has 1 tuning parameter(s):

- blur_sigmas: Gaussian Blur std. dev.s (type: double, default: NULL)

Examples

```
topos <- data.frame(pix = I(list(volcano)))

blur_rec <- recipe(~ ., data = topos) %>% step_blur(pix)
blur_prep <- prep(blur_rec, training = topos)
blur_res <- bake(blur_prep, topos)

tidy(blur_rec, number = 1)
tidy(blur_prep, number = 1)

with_sigmas <- recipe(~ ., data = topos) %>% step_blur(pix, blur_sigmas = 10)
with_sigmas <- bake(prep(with_sigmas, training = topos), topos)

ops <- par(mfrow = c(1, 3))
image(topos$pix[[1]])
image(blur_res$pix[[1]])
image(with_sigmas$pix[[1]])
par(ops)
```

step_pd_degree

Separate persistent pairs by homological degree

Description

The function `step_pd_degree()` creates a *specification* of a recipe step that will separate data sets of persistent pairs by homological degree. The input and output must be list-columns.

Usage

```
step_pd_degree(
  recipe,
  ...,
  role = NA_character_,
  trained = FALSE,
  hom_degrees = NULL,
  columns = NULL,
  keep_original_cols = FALSE,
  skip = FALSE,
  id = rand_id("pd_degree")
)
```

Arguments

recipe	A recipe object. The step will be added to the sequence of operations for this recipe.
...	One or more selector functions to choose variables for this step. See selections() for more details.
role	For model terms created by this step, what analysis role should they be assigned? By default, the new columns created by this step from the original variables will be used as <i>predictors</i> in a model.
trained	A logical to indicate if the quantities for preprocessing have been estimated.
hom_degrees	Integer vector of homological degrees.
columns	A character string of the selected variable names. This field is a placeholder and will be populated once prep() is used.
keep_original_cols	A logical to keep the original variables in the output. Defaults to FALSE.
skip	A logical. Should the step be skipped when the recipe is baked by bake() ? While all operations are baked when prep() is run, some operations may not be able to be conducted on new data (e.g. processing the outcome variable(s)). Care should be taken when using <code>skip = TRUE</code> as it may affect the computations for subsequent operations.
id	A character string that is unique to this step to identify it.

Details

The `hom_degrees` argument sets the homological degrees for which to return new list-columns. If not NULL (the default), it is intersected with the degrees found in any specified columns of the training data; otherwise all found degrees are used. This parameter cannot be tuned.

Value

An updated version of `recipe` with the new step added to the sequence of any existing operations.

See Also

Other topological feature extraction via persistent homology: [step_pd_point_cloud\(\)](#), [step_pd_raster\(\)](#)

Examples

```
dat <- data.frame(
  roads = I(list(eurodist, UScitiesD * 1.6)),
  topos = I(list(volcano, 255 - volcano))
)

ph_rec <- recipe(~ ., data = dat) %>%
  step_pd_point_cloud(roads) %>%
  step_pd_raster(topos) %>%
  step_pd_degree(roads, topos)
ph_prep <- prep(ph_rec, training = dat)
```

```
(ph_res <- bake(ph_prep, dat))

tidy(ph_rec, number = 3)
tidy(ph_prep, number = 3)

with_degs <- recipe(~ ., data = dat) %>%
  step_pd_point_cloud(roads) %>%
  step_pd_raster(topos) %>%
  step_pd_degree(roads, topos, hom_degrees = c(1, 2))
with_degs <- prep(with_degs, training = dat)
bake(with_degs, dat)
```

step_pd_point_cloud *Persistent homology of point clouds*

Description

The function `step_pd_point_cloud()` creates a *specification* of a recipe step that will convert compatible data formats (distance matrices, coordinate matrices, or time series) to 3-column matrix representations of persistence diagram data. The input and output must be list-columns.

Usage

```
step_pd_point_cloud(
  recipe,
  ...,
  role = NA_character_,
  trained = FALSE,
  filtration = "Rips",
  max_hom_degree = 1L,
  radius_max = NULL,
  diameter_max = NULL,
  field_order = 2L,
  engine = NULL,
  columns = NULL,
  skip = FALSE,
  id = rand_id("pd_point_cloud")
)
```

Arguments

<code>recipe</code>	A recipe object. The step will be added to the sequence of operations for this recipe.
<code>...</code>	One or more selector functions to choose variables for this step. See selections() for more details.
<code>role</code>	For model terms created by this step, what analysis role should they be assigned? By default, the new columns created by this step from the original variables will be used as <i>predictors</i> in a model.

trained	A logical to indicate if the quantities for preprocessing have been estimated.
filtration	The type of filtration from which to compute persistent homology; one of "Rips", "Vietoris" (equivalent), or "alpha".
max_hom_degree, radius_max, diameter_max, field_order	Parameters passed to persistence engines.
engine	The computational engine to use (see 'Details'). Reasonable defaults are chosen based on filtration.
columns	A character string of the selected variable names. This field is a placeholder and will be populated once <code>prep()</code> is used.
skip	A logical. Should the step be skipped when the recipe is baked by <code>bake()</code> ? While all operations are baked when <code>prep()</code> is run, some operations may not be able to be conducted on new data (e.g. processing the outcome variable(s)). Care should be taken when using <code>skip = TRUE</code> as it may affect the computations for subsequent operations.
id	A character string that is unique to this step to identify it.

Details

Persistent homology (PH) is a tool of algebraic topology to extract features from data whose *persistence* measures their robustness to scale. The computation relies on a sequence of maps between discrete topological spaces (usually a filtration comprising only inclusions) constructed from the data.

Value

An updated version of recipe with the new step added to the sequence of any existing operations.

PH of Point Clouds

The PH of a point cloud arises from a simplicial filtration (usually Vietoris–Rips, Čech, or alpha) along an increasing distance threshold.

Ripsper is a highly efficient implementation of PH on a point cloud (a finite metric space) via the Vietoris–Rips filtration and is ported to R through `ripserr`. **TDA** calls the Dionysus, PHAT, and GUDHI libraries to compute PH via Vietoris–Rips and alpha filtrations. The `filtration` parameter controls the choice of filtration while the `engine` parameter allows the user to manually select an implementation.

Both engines accept data sets in distance matrix, coordinate matrix, data frame, and time series formats.

The `max_hom_degree` argument determines the highest-dimensional features to be calculated. Either `diameter_max` (preferred) or `radius_max` can be used to bound the distance threshold along which PH is computed. The `field_order` argument should be prime and will be the order of the field of coefficients used in the computation. In most applications, only `max_hom_degree` will be tuned, and to at most 3L.

Tuning Parameters

This step has 1 tuning parameter(s):

- `max_hom_degree`: Maximum Homological Degree (type: integer, default: 1)

See Also

Other topological feature extraction via persistent homology: [step_pd_degree\(\)](#), [step_pd_raster\(\)](#)

Examples

```
roads <- data.frame(dist = I(list(eurodist, UScitiesD * 1.6)))

ph_rec <- recipe(~ ., data = roads) %>%
  step_pd_point_cloud(dist, max_hom_degree = 1, filtration = "Rips")
ph_prep <- prep(ph_rec, training = roads)
ph_res <- bake(ph_prep, roads)

tidy(ph_rec, number = 1)
tidy(ph_prep, number = 1)

ops <- par(mfrow = c(1, 2), mar = c(2, 2, 0, 0) + 0.1)
for (i in seq(nrow(ph_res))) {
  with(ph_res$dist[[i]], plot(
    x = birth, y = death, pch = dimension + 1, col = dimension + 1,
    xlab = NA, ylab = "", asp = 1
  ))
}
par(ops)

with_max <- recipe(~ ., data = roads) %>%
  step_pd_point_cloud(dist, max_hom_degree = 1, diameter_max = 200)
with_max <- prep(with_max, training = roads)
bake(with_max, roads)
```

step_pd_raster

Persistent homology of raster data (images)

Description

The function `step_pd_raster()` creates a *specification* of a recipe step that will convert compatible data formats (numerical arrays, including matrices, of 2, 3, or 4 dimensions) to 3-column matrix representations of persistence diagram data. The input and output must be list-columns.

Usage

```
step_pd_raster(
  recipe,
  ...,
```

```

    role = NA_character_,
    trained = FALSE,
    filtration = "cubical",
    value_max = 9999L,
    method = c("link_join", "compute_pairs"),
    engine = NULL,
    columns = NULL,
    skip = FALSE,
    id = rand_id("pd_raster")
  )

```

Arguments

recipe	A recipe object. The step will be added to the sequence of operations for this recipe.
...	One or more selector functions to choose variables for this step. See selections() for more details.
role	For model terms created by this step, what analysis role should they be assigned? By default, the new columns created by this step from the original variables will be used as <i>predictors</i> in a model.
trained	A logical to indicate if the quantities for preprocessing have been estimated.
filtration	The type of filtration from which to compute persistent homology; currently only "cubical".
value_max, method	Parameters passed to persistence engines.
engine	The computational engine to use (see 'Details'). Reasonable defaults are chosen based on filtration.
columns	A character string of the selected variable names. This field is a placeholder and will be populated once prep() is used.
skip	A logical. Should the step be skipped when the recipe is baked by bake() ? While all operations are baked when prep() is run, some operations may not be able to be conducted on new data (e.g. processing the outcome variable(s)). Care should be taken when using <code>skip = TRUE</code> as it may affect the computations for subsequent operations.
id	A character string that is unique to this step to identify it.

Details

Persistent homology (PH) is a tool of algebraic topology to extract features from data whose *persistence* measures their robustness to scale. The computation relies on a sequence of maps between discrete topological spaces (usually a filtration comprising only inclusions) constructed from the data.

Value

An updated version of recipe with the new step added to the sequence of any existing operations.

PH of Rasters

The PH of numeric arrays such as (greyscale) digital images is computed from the cubical filtration of the pixel or voxel array, treated as a function from a cubical mesh to a finite value range.

Cubical Ripser is an efficient implementation of cubical PH and is ported to R through [ripserr](#). It accepts numerical arrays.

The `value_max` argument bounds the value range along which PH is computed. Cubical Ripser is implemented using both of two methods, link-join and compute-pairs, controlled by the `method` parameter.

Tuning Parameters

This step has 1 tuning parameter(s):

- `max_hom_degree`: Maximum Homological Degree (type: integer, default: NULL)

See Also

Other topological feature extraction via persistent homology: [step_pd_degree\(\)](#), [step_pd_point_cloud\(\)](#)

Examples

```
topos <- data.frame(pix = I(list(volcano)))

ph_rec <- recipe(~ ., data = topos) %>%
  step_pd_raster(pix)
ph_prep <- prep(ph_rec, training = topos)
ph_res <- bake(ph_prep, topos)

tidy(ph_rec, number = 1)
tidy(ph_prep, number = 1)

with(ph_res$pix[[1]], plot(
  x = birth, y = death, pch = dimension + 1, col = dimension + 1,
  xlab = NA, ylab = "", asp = 1
))

with_max <- recipe(~ ., data = topos) %>%
  step_pd_raster(pix, value_max = 150)
with_max <- prep(with_max, training = topos)
bake(with_max, topos)
```

Description

The function `step_vpd_algebraic_functions()` creates a *specification* of a recipe step that will convert a list-column of 3-column matrices of persistence data to a list-column of 1-row matrices of vectorizations.

Usage

```
step_vpd_algebraic_functions(
  recipe,
  ...,
  role = "predictor",
  trained = FALSE,
  hom_degree = 0L,
  columns = NULL,
  keep_original_cols = TRUE,
  skip = FALSE,
  id = rand_id("vpd_algebraic_functions")
)
```

Arguments

<code>recipe</code>	A recipe object. The step will be added to the sequence of operations for this recipe.
<code>...</code>	One or more selector functions to choose variables for this step. See selections() for more details.
<code>role</code>	For model terms created by this step, what analysis role should they be assigned? By default, the new columns created by this step from the original variables will be used as <i>predictors</i> in a model.
<code>trained</code>	A logical to indicate if the quantities for preprocessing have been estimated.
<code>hom_degree</code>	The homological degree of the features to be transformed.
<code>columns</code>	A character string of the selected variable names. This field is a placeholder and will be populated once prep() is used.
<code>keep_original_cols</code>	A logical to keep the original variables in the output. Defaults to FALSE.
<code>skip</code>	A logical. Should the step be skipped when the recipe is baked by bake() ? While all operations are baked when prep() is run, some operations may not be able to be conducted on new data (e.g. processing the outcome variable(s)). Care should be taken when using <code>skip = TRUE</code> as it may affect the computations for subsequent operations.
<code>id</code>	A character string that is unique to this step to identify it.

Details

Persistent homology is usually encoded as birth–death pairs (barcodes or diagrams), but the space of persistence data sets does not satisfy convenient statistical properties. Such applications as hypothesis testing and machine learning benefit from transformations of persistence data, often to Hilbert spaces (vector spaces with inner products and induced metrics).

Value

An updated version of recipe with the new step added to the sequence of any existing operations.

Engine

The algebraic functions vectorization deploys `TDAvec::computeAlgebraicFunctions()`. See there for definitions and references.

Tuning Parameters

This step has 1 tuning parameter:

- `hom_degree`: Homological degree (type: integer, default: 0L)

Examples

```
library(recipes)

# inspect vectorized features
volc_dat <- data.frame(image = I(list(volcano / 10)))
recipe(~ image, data = volc_dat) %>%
  step_pd_raster(image, method = "link_join") %>%
  step_vpd_algebraic_functions(image, hom_degree = 1) %>%
  print() -> volc_rec
print(volc_rec)
volc_rec %>%
  prep(training = volc_dat) %>%
  bake(new_data = volc_dat)

# dimension-reduce using vectorized features
data(permeability_qsar, package = "modeldata")
permeability_qsar %>%
  transform(perm_cut = cut(permeability, breaks = seq(0, 60, 10))) %>%
  subset(select = -permeability) %>%
  tidyr::nest(chem_fp = -perm_cut) %>%
  print() -> perm_dat
recipe(perm_cut ~ chem_fp, data = perm_dat) %>%
  step_pd_point_cloud(chem_fp, max_hom_degree = 2) %>%
  step_vpd_algebraic_functions(chem_fp, hom_degree = 1) %>%
  step_pca(starts_with("chem_fp_"), num_comp = 2) %>%
  print() -> perm_rec
perm_est <- prep(perm_rec, training = perm_dat)
perm_res <- bake(perm_est, new_data = perm_dat)
# inspect results
tidy(perm_rec)
tidy(perm_rec, number = 2)
tidy(perm_est, number = 2)
# visualize results
with(perm_res, {
  plot(PC1, PC2, type = "n", asp = 1)
  text(PC1, PC2, labels = perm_cut)
})
```

 step_vpd_betti_curve *Betti Curve Vectorization of Persistent Homology*

Description

The function `step_vpd_betti_curve()` creates a *specification* of a recipe step that will convert a list-column of 3-column matrices of persistence data to a list-column of 1-row matrices of vectorizations.

Usage

```
step_vpd_betti_curve(
  recipe,
  ...,
  role = "predictor",
  trained = FALSE,
  hom_degree = 0L,
  xseq = NULL,
  xmin = NULL,
  xmax = NULL,
  xlen = NULL,
  xby = NULL,
  evaluate = "intervals",
  columns = NULL,
  keep_original_cols = TRUE,
  skip = FALSE,
  id = rand_id("vpd_betti_curve")
)
```

Arguments

<code>recipe</code>	A recipe object. The step will be added to the sequence of operations for this recipe.
<code>...</code>	One or more selector functions to choose variables for this step. See selections() for more details.
<code>role</code>	For model terms created by this step, what analysis role should they be assigned? By default, the new columns created by this step from the original variables will be used as <i>predictors</i> in a model.
<code>trained</code>	A logical to indicate if the quantities for preprocessing have been estimated.
<code>hom_degree</code>	The homological degree of the features to be transformed.
<code>xseq</code>	A discretization grid, as an increasing numeric vector. <code>xseq</code> overrides the other <code>x*</code> parameters with a warning.
<code>xmin, xmax, xlen, xby</code>	Limits and resolution of a discretization grid; specify only one of <code>xlen</code> and <code>xby</code> .

evaluate	The method by which to vectorize continuous functions over a grid, either 'intervals' or 'points'. Some functions only admit one method.
columns	A character string of the selected variable names. This field is a placeholder and will be populated once <code>prep()</code> is used.
keep_original_cols	A logical to keep the original variables in the output. Defaults to FALSE.
skip	A logical. Should the step be skipped when the recipe is baked by <code>bake()</code> ? While all operations are baked when <code>prep()</code> is run, some operations may not be able to be conducted on new data (e.g. processing the outcome variable(s)). Care should be taken when using <code>skip = TRUE</code> as it may affect the computations for subsequent operations.
id	A character string that is unique to this step to identify it.

Details

Persistent homology is usually encoded as birth–death pairs (barcodes or diagrams), but the space of persistence data sets does not satisfy convenient statistical properties. Such applications as hypothesis testing and machine learning benefit from transformations of persistence data, often to Hilbert spaces (vector spaces with inner products and induced metrics).

Value

An updated version of recipe with the new step added to the sequence of any existing operations.

Engine

The Betti curve vectorization deploys `TDAvec::computeBettiCurve()`. See there for definitions and references.

Tuning Parameters

This step has 1 tuning parameter:

- `hom_degree`: Homological degree (type: integer, default: 0L)

Examples

```
library(recipes)

# inspect vectorized features
volc_dat <- data.frame(image = I(list(volcano / 10)))
recipe(~ image, data = volc_dat) %>%
  step_pd_raster(image, method = "link_join") %>%
  step_vpd_betti_curve(image, hom_degree = 1) %>%
  print() -> volc_rec
print(volc_rec)
volc_rec %>%
  prep(training = volc_dat) %>%
  bake(new_data = volc_dat)
```

```

# dimension-reduce using vectorized features
data(permeability_qsar, package = "modeldata")
permeability_qsar %>%
  transform(perm_cut = cut(permeability, breaks = seq(0, 60, 10))) %>%
  subset(select = -permeability) %>%
  tidyr::nest(chem_fp = -perm_cut) %>%
  print() -> perm_dat
recipe(perm_cut ~ chem_fp, data = perm_dat) %>%
  step_pd_point_cloud(chem_fp, max_hom_degree = 2) %>%
  step_vpd_betti_curve(chem_fp, hom_degree = 1) %>%
  step_pca(starts_with("chem_fp_"), num_comp = 2) %>%
  print() -> perm_rec
perm_est <- prep(perm_rec, training = perm_dat)
perm_res <- bake(perm_est, new_data = perm_dat)
# inspect results
tidy(perm_rec)
tidy(perm_rec, number = 2)
tidy(perm_est, number = 2)
# visualize results
with(perm_res, {
  plot(PC1, PC2, type = "n", asp = 1)
  text(PC1, PC2, labels = perm_cut)
})

```

step_vpd_complex_polynomial

Complex Polynomial Vectorization of Persistent Homology

Description

The function `step_vpd_complex_polynomial()` creates a *specification* of a recipe step that will convert a list-column of 3-column matrices of persistence data to a list-column of 1-row matrices of vectorizations.

Usage

```

step_vpd_complex_polynomial(
  recipe,
  ...,
  role = "predictor",
  trained = FALSE,
  hom_degree = 0L,
  num_coef = 1L,
  poly_type = "R",
  columns = NULL,
  keep_original_cols = TRUE,
  skip = FALSE,
  id = rand_id("vpd_complex_polynomial")
)

```

Arguments

recipe	A recipe object. The step will be added to the sequence of operations for this recipe.
...	One or more selector functions to choose variables for this step. See selections() for more details.
role	For model terms created by this step, what analysis role should they be assigned? By default, the new columns created by this step from the original variables will be used as <i>predictors</i> in a model.
trained	A logical to indicate if the quantities for preprocessing have been estimated.
hom_degree	The homological degree of the features to be transformed.
num_coef	The number of coefficients of a convex polynomial fitted to finite persistence pairs.
poly_type	The type of complex polynomial to fit ('R', 'S', or 'T').
columns	A character string of the selected variable names. This field is a placeholder and will be populated once prep() is used.
keep_original_cols	A logical to keep the original variables in the output. Defaults to FALSE.
skip	A logical. Should the step be skipped when the recipe is baked by bake() ? While all operations are baked when prep() is run, some operations may not be able to be conducted on new data (e.g. processing the outcome variable(s)). Care should be taken when using <code>skip = TRUE</code> as it may affect the computations for subsequent operations.
id	A character string that is unique to this step to identify it.

Details

Persistent homology is usually encoded as birth–death pairs (barcodes or diagrams), but the space of persistence data sets does not satisfy convenient statistical properties. Such applications as hypothesis testing and machine learning benefit from transformations of persistence data, often to Hilbert spaces (vector spaces with inner products and induced metrics).

Value

An updated version of recipe with the new step added to the sequence of any existing operations.

Engine

The complex polynomial vectorization deploys `TDavec::computeComplexPolynomial()`. See there for definitions and references.

Tuning Parameters

This step has 3 tuning parameters:

- `hom_degree`: Homological degree (type: integer, default: 0L)
- `num_coef`: # Polynomial coefficients (type: integer, default: 1L)
- `poly_type`: Type of polynomial (type: character, default: "R")

Examples

```

library(recipes)

# inspect vectorized features
volc_dat <- data.frame(image = I(list(volcano / 10)))
recipe(~ image, data = volc_dat) %>%
  step_pd_raster(image, method = "link_join") %>%
  step_vpd_complex_polynomial(image, hom_degree = 1) %>%
  print() -> volc_rec
print(volc_rec)
volc_rec %>%
  prep(training = volc_dat) %>%
  bake(new_data = volc_dat)

# dimension-reduce using vectorized features
data(permeability_qsar, package = "modeldata")
permeability_qsar %>%
  transform(perm_cut = cut(permeability, breaks = seq(0, 60, 10))) %>%
  subset(select = -permeability) %>%
  tidyr::nest(chem_fp = -perm_cut) %>%
  print() -> perm_dat
recipe(perm_cut ~ chem_fp, data = perm_dat) %>%
  step_pd_point_cloud(chem_fp, max_hom_degree = 2) %>%
  step_vpd_complex_polynomial(chem_fp, hom_degree = 1) %>%
  step_pca(starts_with("chem_fp_"), num_comp = 2) %>%
  print() -> perm_rec
perm_est <- prep(perm_rec, training = perm_dat)
perm_res <- bake(perm_est, new_data = perm_dat)
# inspect results
tidy(perm_rec)
tidy(perm_rec, number = 2)
tidy(perm_est, number = 2)
# visualize results
with(perm_res, {
  plot(PC1, PC2, type = "n", asp = 1)
  text(PC1, PC2, labels = perm_cut)
})

```

step_vpd_descriptive_statistics

Descriptive Statistics Vectorization of Persistent Homology

Description

The function `step_vpd_descriptive_statistics()` creates a *specification* of a recipe step that will convert a list-column of 3-column matrices of persistence data to a list-column of 1-row matrices of vectorizations.

Usage

```
step_vpd_descriptive_statistics(
  recipe,
  ...,
  role = "predictor",
  trained = FALSE,
  hom_degree = 0L,
  columns = NULL,
  keep_original_cols = TRUE,
  skip = FALSE,
  id = rand_id("vpd_descriptive_statistics")
)
```

Arguments

recipe	A recipe object. The step will be added to the sequence of operations for this recipe.
...	One or more selector functions to choose variables for this step. See selections() for more details.
role	For model terms created by this step, what analysis role should they be assigned? By default, the new columns created by this step from the original variables will be used as <i>predictors</i> in a model.
trained	A logical to indicate if the quantities for preprocessing have been estimated.
hom_degree	The homological degree of the features to be transformed.
columns	A character string of the selected variable names. This field is a placeholder and will be populated once prep() is used.
keep_original_cols	A logical to keep the original variables in the output. Defaults to FALSE.
skip	A logical. Should the step be skipped when the recipe is baked by bake() ? While all operations are baked when prep() is run, some operations may not be able to be conducted on new data (e.g. processing the outcome variable(s)). Care should be taken when using <code>skip = TRUE</code> as it may affect the computations for subsequent operations.
id	A character string that is unique to this step to identify it.

Details

Persistent homology is usually encoded as birth–death pairs (barcodes or diagrams), but the space of persistence data sets does not satisfy convenient statistical properties. Such applications as hypothesis testing and machine learning benefit from transformations of persistence data, often to Hilbert spaces (vector spaces with inner products and induced metrics).

Value

An updated version of recipe with the new step added to the sequence of any existing operations.

Engine

The descriptive statistics vectorization deploys `TDavec::computeStats()`. See there for definitions and references.

Tuning Parameters

This step has 1 tuning parameter:

- `hom_degree`: Homological degree (type: integer, default: 0L)

Examples

```
library(recipes)

# inspect vectorized features
volc_dat <- data.frame(image = I(list(volcano / 10)))
recipe(~ image, data = volc_dat) %>%
  step_pd_raster(image, method = "link_join") %>%
  step_vpd_descriptive_statistics(image, hom_degree = 1) %>%
  print() -> volc_rec
print(volc_rec)
volc_rec %>%
  prep(training = volc_dat) %>%
  bake(new_data = volc_dat)

# dimension-reduce using vectorized features
data(permeability_qsar, package = "modeldata")
permeability_qsar %>%
  transform(perm_cut = cut(permeability, breaks = seq(0, 60, 10))) %>%
  subset(select = -permeability) %>%
  tidyr::nest(chem_fp = -perm_cut) %>%
  print() -> perm_dat
recipe(perm_cut ~ chem_fp, data = perm_dat) %>%
  step_pd_point_cloud(chem_fp, max_hom_degree = 2) %>%
  step_vpd_descriptive_statistics(chem_fp, hom_degree = 1) %>%
  step_pca(starts_with("chem_fp_"), num_comp = 2) %>%
  print() -> perm_rec
perm_est <- prep(perm_rec, training = perm_dat)
perm_res <- bake(perm_est, new_data = perm_dat)
# inspect results
tidy(perm_rec)
tidy(perm_rec, number = 2)
tidy(perm_est, number = 2)
# visualize results
with(perm_res, {
  plot(PC1, PC2, type = "n", asp = 1)
  text(PC1, PC2, labels = perm_cut)
})
```

 step_vpd_euler_characteristic_curve

Euler Characteristic Curve Vectorization of Persistent Homology

Description

The function `step_vpd_euler_characteristic_curve()` creates a *specification* of a recipe step that will convert a list-column of 3-column matrices of persistence data to a list-column of 1-row matrices of vectorizations.

Usage

```
step_vpd_euler_characteristic_curve(
  recipe,
  ...,
  role = "predictor",
  trained = FALSE,
  xseq = NULL,
  xmin = NULL,
  xmax = NULL,
  xlen = NULL,
  xby = NULL,
  max_hom_degree = Inf,
  evaluate = "intervals",
  columns = NULL,
  keep_original_cols = TRUE,
  skip = FALSE,
  id = rand_id("vpd_euler_characteristic_curve")
)
```

Arguments

<code>recipe</code>	A recipe object. The step will be added to the sequence of operations for this recipe.
<code>...</code>	One or more selector functions to choose variables for this step. See selections() for more details.
<code>role</code>	For model terms created by this step, what analysis role should they be assigned? By default, the new columns created by this step from the original variables will be used as <i>predictors</i> in a model.
<code>trained</code>	A logical to indicate if the quantities for preprocessing have been estimated.
<code>xseq</code>	A discretization grid, as an increasing numeric vector. <code>xseq</code> overrides the other <code>x*</code> parameters with a warning.
<code>xmin, xmax, xlen, xby</code>	Limits and resolution of a discretization grid; specify only one of <code>xlen</code> and <code>xby</code> .
<code>max_hom_degree</code>	The highest degree, starting from 0, of the features to be transformed.

evaluate	The method by which to vectorize continuous functions over a grid, either 'intervals' or 'points'. Some functions only admit one method.
columns	A character string of the selected variable names. This field is a placeholder and will be populated once <code>prep()</code> is used.
keep_original_cols	A logical to keep the original variables in the output. Defaults to FALSE.
skip	A logical. Should the step be skipped when the recipe is baked by <code>bake()</code> ? While all operations are baked when <code>prep()</code> is run, some operations may not be able to be conducted on new data (e.g. processing the outcome variable(s)). Care should be taken when using <code>skip = TRUE</code> as it may affect the computations for subsequent operations.
id	A character string that is unique to this step to identify it.

Details

Persistent homology is usually encoded as birth–death pairs (barcodes or diagrams), but the space of persistence data sets does not satisfy convenient statistical properties. Such applications as hypothesis testing and machine learning benefit from transformations of persistence data, often to Hilbert spaces (vector spaces with inner products and induced metrics).

Value

An updated version of recipe with the new step added to the sequence of any existing operations.

Engine

The Euler characteristic curve vectorization deploys `TDavec::computeEulerCharacteristic()`. See there for definitions and references.

Tuning Parameters

This step has 1 tuning parameter:

- `max_hom_degree`: Highest homological degree (type: integer, default: Inf)

Examples

```
library(recipes)

# inspect vectorized features
volc_dat <- data.frame(image = I(list(volcano / 10)))
recipe(~ image, data = volc_dat) %>%
  step_pd_raster(image, method = "link_join") %>%
  step_vpd_euler_characteristic_curve(image, max_hom_degree = 2) %>%
  print() -> volc_rec
print(volc_rec)
volc_rec %>%
  prep(training = volc_dat) %>%
  bake(new_data = volc_dat)
```

```

# dimension-reduce using vectorized features
data(permeability_qsar, package = "modeldata")
permeability_qsar %>%
  transform(perm_cut = cut(permeability, breaks = seq(0, 60, 10))) %>%
  subset(select = -permeability) %>%
  tidyr::nest(chem_fp = -perm_cut) %>%
  print() -> perm_dat
recipe(perm_cut ~ chem_fp, data = perm_dat) %>%
  step_pd_point_cloud(chem_fp, max_hom_degree = 2) %>%
  step_vpd_euler_characteristic_curve(chem_fp, max_hom_degree = 2) %>%
  step_pca(starts_with("chem_fp_"), num_comp = 2) %>%
  print() -> perm_rec
perm_est <- prep(perm_rec, training = perm_dat)
perm_res <- bake(perm_est, new_data = perm_dat)
# inspect results
tidy(perm_rec)
tidy(perm_rec, number = 2)
tidy(perm_est, number = 2)
# visualize results
with(perm_res, {
  plot(PC1, PC2, type = "n", asp = 1)
  text(PC1, PC2, labels = perm_cut)
})

```

```
step_vpd_normalized_life_curve
```

Normalized Life Curve Vectorization of Persistent Homology

Description

The function `step_vpd_normalized_life_curve()` creates a *specification* of a recipe step that will convert a list-column of 3-column matrices of persistence data to a list-column of 1-row matrices of vectorizations.

Usage

```

step_vpd_normalized_life_curve(
  recipe,
  ...,
  role = "predictor",
  trained = FALSE,
  hom_degree = 0L,
  xseq = NULL,
  xmin = NULL,
  xmax = NULL,
  xlen = NULL,
  xby = NULL,
  evaluate = "intervals",
  columns = NULL,

```

```

    keep_original_cols = TRUE,
    skip = FALSE,
    id = rand_id("vpd_normalized_life_curve")
  )

```

Arguments

recipe	A recipe object. The step will be added to the sequence of operations for this recipe.
...	One or more selector functions to choose variables for this step. See selections() for more details.
role	For model terms created by this step, what analysis role should they be assigned? By default, the new columns created by this step from the original variables will be used as <i>predictors</i> in a model.
trained	A logical to indicate if the quantities for preprocessing have been estimated.
hom_degree	The homological degree of the features to be transformed.
xseq	A discretization grid, as an increasing numeric vector. xseq overrides the other x* parameters with a warning.
xmin, xmax, xlen, xby	Limits and resolution of a discretization grid; specify only one of xlen and xby.
evaluate	The method by which to vectorize continuous functions over a grid, either 'intervals' or 'points'. Some functions only admit one method.
columns	A character string of the selected variable names. This field is a placeholder and will be populated once prep() is used.
keep_original_cols	A logical to keep the original variables in the output. Defaults to FALSE.
skip	A logical. Should the step be skipped when the recipe is baked by bake() ? While all operations are baked when prep() is run, some operations may not be able to be conducted on new data (e.g. processing the outcome variable(s)). Care should be taken when using skip = TRUE as it may affect the computations for subsequent operations.
id	A character string that is unique to this step to identify it.

Details

Persistent homology is usually encoded as birth–death pairs (barcodes or diagrams), but the space of persistence data sets does not satisfy convenient statistical properties. Such applications as hypothesis testing and machine learning benefit from transformations of persistence data, often to Hilbert spaces (vector spaces with inner products and induced metrics).

Value

An updated version of recipe with the new step added to the sequence of any existing operations.

Engine

The normalized life curve vectorization deploys `TDavec::computeNormalizedLife()`. See there for definitions and references.

Tuning Parameters

This step has 1 tuning parameter:

- `hom_degree`: Homological degree (type: integer, default: 0L)

Examples

```
library(recipes)

# inspect vectorized features
volc_dat <- data.frame(image = I(list(volcano / 10)))
recipe(~ image, data = volc_dat) %>%
  step_pd_raster(image, method = "link_join") %>%
  step_vpd_normalized_life_curve(image, hom_degree = 1) %>%
  print() -> volc_rec
print(volc_rec)
volc_rec %>%
  prep(training = volc_dat) %>%
  bake(new_data = volc_dat)

# dimension-reduce using vectorized features
data(permeability_qsar, package = "modeldata")
permeability_qsar %>%
  transform(perm_cut = cut(permeability, breaks = seq(0, 60, 10))) %>%
  subset(select = -permeability) %>%
  tidyr::nest(chem_fp = -perm_cut) %>%
  print() -> perm_dat
recipe(perm_cut ~ chem_fp, data = perm_dat) %>%
  step_pd_point_cloud(chem_fp, max_hom_degree = 2) %>%
  step_vpd_normalized_life_curve(chem_fp, hom_degree = 1) %>%
  step_pca(starts_with("chem_fp_"), num_comp = 2) %>%
  print() -> perm_rec
perm_est <- prep(perm_rec, training = perm_dat)
perm_res <- bake(perm_est, new_data = perm_dat)
# inspect results
tidy(perm_rec)
tidy(perm_rec, number = 2)
tidy(perm_est, number = 2)
# visualize results
with(perm_res, {
  plot(PC1, PC2, type = "n", asp = 1)
  text(PC1, PC2, labels = perm_cut)
})
```

step_vpd_persistence_block

Persistence Block Vectorization of Persistent Homology

Description

The function `step_vpd_persistence_block()` creates a *specification* of a recipe step that will convert a list-column of 3-column matrices of persistence data to a list-column of 1-row matrices of vectorizations.

Usage

```
step_vpd_persistence_block(
  recipe,
  ...,
  role = "predictor",
  trained = FALSE,
  hom_degree = 0L,
  xseq = NULL,
  xmin = NULL,
  xmax = NULL,
  xlen = NULL,
  xby = NULL,
  yseq = NULL,
  ymin = NULL,
  ymax = NULL,
  ylen = NULL,
  yby = NULL,
  block_size = 0.3,
  columns = NULL,
  keep_original_cols = TRUE,
  skip = FALSE,
  id = rand_id("vpd_persistence_block")
)
```

Arguments

<code>recipe</code>	A recipe object. The step will be added to the sequence of operations for this recipe.
<code>...</code>	One or more selector functions to choose variables for this step. See selections() for more details.
<code>role</code>	For model terms created by this step, what analysis role should they be assigned? By default, the new columns created by this step from the original variables will be used as <i>predictors</i> in a model.
<code>trained</code>	A logical to indicate if the quantities for preprocessing have been estimated.
<code>hom_degree</code>	The homological degree of the features to be transformed.
<code>xseq</code>	A discretization grid, as an increasing numeric vector. <code>xseq</code> overrides the other <code>x*</code> parameters with a warning.
<code>xmin, xmax, xlen, xby</code>	Limits and resolution of a discretization grid; specify only one of <code>xlen</code> and <code>xby</code> .
<code>yseq</code>	Combined with <code>xseq</code> to form a 2-dimensional discretization grid.

ymin, ymax, ylen, yby	Limits and resolution of a discretization grid; specify only one of ylen and yby.
block_size	The scaling factor of the squares used to obtain persistence blocks. The side length of the square centered at a feature (b, p) is obtained by multiplying $2p$ by this factor.
columns	A character string of the selected variable names. This field is a placeholder and will be populated once <code>prep()</code> is used.
keep_original_cols	A logical to keep the original variables in the output. Defaults to FALSE.
skip	A logical. Should the step be skipped when the recipe is baked by <code>bake()</code> ? While all operations are baked when <code>prep()</code> is run, some operations may not be able to be conducted on new data (e.g. processing the outcome variable(s)). Care should be taken when using <code>skip = TRUE</code> as it may affect the computations for subsequent operations.
id	A character string that is unique to this step to identify it.

Details

Persistent homology is usually encoded as birth–death pairs (barcodes or diagrams), but the space of persistence data sets does not satisfy convenient statistical properties. Such applications as hypothesis testing and machine learning benefit from transformations of persistence data, often to Hilbert spaces (vector spaces with inner products and induced metrics).

Value

An updated version of recipe with the new step added to the sequence of any existing operations.

Engine

The persistence block vectorization deploys `TDAvec::computePersistenceBlock()`. See there for definitions and references.

Tuning Parameters

This step has 2 tuning parameters:

- `hom_degree`: Homological degree (type: integer, default: 0L)
- `block_size`: Square side length scaling factor (type: double, default: 0.3)

Examples

```
library(recipes)

# inspect vectorized features
volc_dat <- data.frame(image = I(list(volcano / 10)))
recipe(~ image, data = volc_dat) %>%
  step_pd_raster(image, method = "link_join") %>%
  step_vpd_persistence_block(image, hom_degree = 1, block_size = 1) %>%
  print() -> volc_rec
```

```

print(volc_rec)
volc_rec %>%
  prep(training = volc_dat) %>%
  bake(new_data = volc_dat)

# dimension-reduce using vectorized features
data(permeability_qsar, package = "modeldata")
permeability_qsar %>%
  transform(perm_cut = cut(permeability, breaks = seq(0, 60, 10))) %>%
  subset(select = -permeability) %>%
  tidyr::nest(chem_fp = -perm_cut) %>%
  print() -> perm_dat
recipe(perm_cut ~ chem_fp, data = perm_dat) %>%
  step_pd_point_cloud(chem_fp, max_hom_degree = 2) %>%
  step_vpd_persistence_block(chem_fp, hom_degree = 1, block_size = 1) %>%
  step_pca(starts_with("chem_fp_"), num_comp = 2) %>%
  print() -> perm_rec
perm_est <- prep(perm_rec, training = perm_dat)
perm_res <- bake(perm_est, new_data = perm_dat)
# inspect results
tidy(perm_rec)
tidy(perm_rec, number = 2)
tidy(perm_est, number = 2)
# visualize results
with(perm_res, {
  plot(PC1, PC2, type = "n", asp = 1)
  text(PC1, PC2, labels = perm_cut)
})

```

step_vpd_persistence_image

Persistence Image Vectorization of Persistent Homology

Description

The function `step_vpd_persistence_image()` creates a *specification* of a recipe step that will convert a list-column of 3-column matrices of persistence data to a list-column of 1-row matrices of vectorizations.

Usage

```

step_vpd_persistence_image(
  recipe,
  ...,
  role = "predictor",
  trained = FALSE,
  hom_degree = 0L,
  xseq = NULL,
  xmin = NULL,

```

```

xmax = NULL,
xlen = NULL,
xby = NULL,
yseq = NULL,
ymin = NULL,
ymax = NULL,
ylen = NULL,
yby = NULL,
img_sigma = 1,
columns = NULL,
keep_original_cols = TRUE,
skip = FALSE,
id = rand_id("vpd_persistence_image")
)

```

Arguments

recipe	A recipe object. The step will be added to the sequence of operations for this recipe.
...	One or more selector functions to choose variables for this step. See selections() for more details.
role	For model terms created by this step, what analysis role should they be assigned? By default, the new columns created by this step from the original variables will be used as <i>predictors</i> in a model.
trained	A logical to indicate if the quantities for preprocessing have been estimated.
hom_degree	The homological degree of the features to be transformed.
xseq	A discretization grid, as an increasing numeric vector. xseq overrides the other x* parameters with a warning.
xmin, xmax, xlen, xby	Limits and resolution of a discretization grid; specify only one of xlen and xby.
yseq	Combined with xseq to form a 2-dimensional discretization grid.
ymin, ymax, ylen, yby	Limits and resolution of a discretization grid; specify only one of ylen and yby.
img_sigma	The standard deviation of the gaussian distribution convolved with persistence diagrams to obtain persistence images.
columns	A character string of the selected variable names. This field is a placeholder and will be populated once prep() is used.
keep_original_cols	A logical to keep the original variables in the output. Defaults to FALSE.
skip	A logical. Should the step be skipped when the recipe is baked by bake() ? While all operations are baked when prep() is run, some operations may not be able to be conducted on new data (e.g. processing the outcome variable(s)). Care should be taken when using skip = TRUE as it may affect the computations for subsequent operations.
id	A character string that is unique to this step to identify it.

Details

Persistent homology is usually encoded as birth–death pairs (barcodes or diagrams), but the space of persistence data sets does not satisfy convenient statistical properties. Such applications as hypothesis testing and machine learning benefit from transformations of persistence data, often to Hilbert spaces (vector spaces with inner products and induced metrics).

Value

An updated version of recipe with the new step added to the sequence of any existing operations.

Engine

The persistence image vectorization deploys `TDavec::computePersistenceImage()`. See there for definitions and references.

Tuning Parameters

This step has 2 tuning parameters:

- `hom_degree`: Homological degree (type: integer, default: 0L)
- `img_sigma`: Convolved Gaussian standard deviation (type: double, default: 1)

Examples

```
library(recipes)

# inspect vectorized features
volc_dat <- data.frame(image = I(list(volcano / 10)))
recipe(~ image, data = volc_dat) %>%
  step_pd_raster(image, method = "link_join") %>%
  step_vpd_persistence_image(image, hom_degree = 1, img_sigma = 1) %>%
  print() -> volc_rec
print(volc_rec)
volc_rec %>%
  prep(training = volc_dat) %>%
  bake(new_data = volc_dat)

# dimension-reduce using vectorized features
data(permeability_qsar, package = "modeldata")
permeability_qsar %>%
  transform(perm_cut = cut(permeability, breaks = seq(0, 60, 10))) %>%
  subset(select = -permeability) %>%
  tidyr::nest(chem_fp = -perm_cut) %>%
  print() -> perm_dat
recipe(perm_cut ~ chem_fp, data = perm_dat) %>%
  step_pd_point_cloud(chem_fp, max_hom_degree = 2) %>%
  step_vpd_persistence_image(chem_fp, hom_degree = 1, img_sigma = 1) %>%
  step_pca(starts_with("chem_fp_"), num_comp = 2) %>%
  print() -> perm_rec
perm_est <- prep(perm_rec, training = perm_dat)
perm_res <- bake(perm_est, new_data = perm_dat)
```

```

# inspect results
tidy(perm_rec)
tidy(perm_rec, number = 2)
tidy(perm_est, number = 2)
# visualize results
with(perm_res, {
  plot(PC1, PC2, type = "n", asp = 1)
  text(PC1, PC2, labels = perm_cut)
})

```

```
step_vpd_persistence_landscape
```

Persistence Landscape Vectorization of Persistent Homology

Description

The function `step_vpd_persistence_landscape()` creates a *specification* of a recipe step that will convert a list-column of 3-column matrices of persistence data to a list-column of 1-row matrices of vectorizations.

Usage

```

step_vpd_persistence_landscape(
  recipe,
  ...,
  role = "predictor",
  trained = FALSE,
  hom_degree = 0L,
  xseq = NULL,
  xmin = NULL,
  xmax = NULL,
  xlen = NULL,
  xby = NULL,
  num_levels = 6L,
  generalized = FALSE,
  weight_func_pl = "triangle",
  bandwidth = NULL,
  columns = NULL,
  keep_original_cols = TRUE,
  skip = FALSE,
  id = rand_id("vpd_persistence_landscape")
)

```

Arguments

<code>recipe</code>	A recipe object. The step will be added to the sequence of operations for this recipe.
---------------------	--

...	One or more selector functions to choose variables for this step. See selections() for more details.
role	For model terms created by this step, what analysis role should they be assigned? By default, the new columns created by this step from the original variables will be used as <i>predictors</i> in a model.
trained	A logical to indicate if the quantities for preprocessing have been estimated.
hom_degree	The homological degree of the features to be transformed.
xseq	A discretization grid, as an increasing numeric vector. <code>xseq</code> overrides the other <code>x*</code> parameters with a warning.
xmin, xmax, xlen, xby	Limits and resolution of a discretization grid; specify only one of <code>xlen</code> and <code>xby</code> .
num_levels	The number of levels of a persistence landscape to vectorize. If <code>num_levels</code> is greater than the length of a landscape, then additional levels of zeros will be included.
generalized	Logical indicator to compute generalized functions.
weight_func_pl	A <i>single</i> character for the type of kernel function used to compute generalized landscapes.
bandwidth	The bandwidth of a kernel function.
columns	A character string of the selected variable names. This field is a placeholder and will be populated once prep() is used.
keep_original_cols	A logical to keep the original variables in the output. Defaults to FALSE.
skip	A logical. Should the step be skipped when the recipe is baked by bake() ? While all operations are baked when prep() is run, some operations may not be able to be conducted on new data (e.g. processing the outcome variable(s)). Care should be taken when using <code>skip = TRUE</code> as it may affect the computations for subsequent operations.
id	A character string that is unique to this step to identify it.

Details

Persistent homology is usually encoded as birth–death pairs (barcodes or diagrams), but the space of persistence data sets does not satisfy convenient statistical properties. Such applications as hypothesis testing and machine learning benefit from transformations of persistence data, often to Hilbert spaces (vector spaces with inner products and induced metrics).

Value

An updated version of recipe with the new step added to the sequence of any existing operations.

Engine

The persistence landscape vectorization deploys `TDAvec::computePersistenceLandscape()`. See there for definitions and references.

Tuning Parameters

This step has 4 tuning parameters:

- `hom_degree`: Homological degree (type: integer, default: 0L)
- `num_levels`: # Levels or envelopes (type: integer, default: 6L)
- `weight_func_pl`: Kernel distance weight function (type: character, default: "triangle")
- `bandwidth`: Kernel bandwidth (type: double, default: NULL)

Examples

```
library(recipes)

# inspect vectorized features
volc_dat <- data.frame(image = I(list(volcano / 10)))
recipe(~ image, data = volc_dat) %>%
  step_pd_raster(image, method = "link_join") %>%
  step_vpd_persistence_landscape(image, hom_degree = 1, num_levels = 3) %>%
  print() -> volc_rec
print(volc_rec)
volc_rec %>%
  prep(training = volc_dat) %>%
  bake(new_data = volc_dat)

# dimension-reduce using vectorized features
data(permeability_qsar, package = "modeldata")
permeability_qsar %>%
  transform(perm_cut = cut(permeability, breaks = seq(0, 60, 10))) %>%
  subset(select = -permeability) %>%
  tidyr::nest(chem_fp = -perm_cut) %>%
  print() -> perm_dat
recipe(perm_cut ~ chem_fp, data = perm_dat) %>%
  step_pd_point_cloud(chem_fp, max_hom_degree = 2) %>%
  step_vpd_persistence_landscape(chem_fp, hom_degree = 1, num_levels = 3) %>%
  step_pca(starts_with("chem_fp"), num_comp = 2) %>%
  print() -> perm_rec
perm_est <- prep(perm_rec, training = perm_dat)
perm_res <- bake(perm_est, new_data = perm_dat)
# inspect results
tidy(perm_rec)
tidy(perm_rec, number = 2)
tidy(perm_est, number = 2)
# visualize results
with(perm_res, {
  plot(PC1, PC2, type = "n", asp = 1)
  text(PC1, PC2, labels = perm_cut)
})
```

 step_vpd_persistence_silhouette

Persistence Silhouette Vectorization of Persistent Homology

Description

The function `step_vpd_persistence_silhouette()` creates a *specification* of a recipe step that will convert a list-column of 3-column matrices of persistence data to a list-column of 1-row matrices of vectorizations.

Usage

```
step_vpd_persistence_silhouette(
  recipe,
  ...,
  role = "predictor",
  trained = FALSE,
  hom_degree = 0L,
  xseq = NULL,
  xmin = NULL,
  xmax = NULL,
  xlen = NULL,
  xby = NULL,
  weight_power = 1,
  evaluate = "intervals",
  columns = NULL,
  keep_original_cols = TRUE,
  skip = FALSE,
  id = rand_id("vpd_persistence_silhouette")
)
```

Arguments

<code>recipe</code>	A recipe object. The step will be added to the sequence of operations for this recipe.
<code>...</code>	One or more selector functions to choose variables for this step. See selections() for more details.
<code>role</code>	For model terms created by this step, what analysis role should they be assigned? By default, the new columns created by this step from the original variables will be used as <i>predictors</i> in a model.
<code>trained</code>	A logical to indicate if the quantities for preprocessing have been estimated.
<code>hom_degree</code>	The homological degree of the features to be transformed.
<code>xseq</code>	A discretization grid, as an increasing numeric vector. <code>xseq</code> overrides the other <code>x*</code> parameters with a warning.

xmin, xmax, xlen, xby	Limits and resolution of a discretization grid; specify only one of xlen and xby.
weight_power	The power of weights in a persistence silhouette function.
evaluate	The method by which to vectorize continuous functions over a grid, either 'intervals' or 'points'. Some functions only admit one method.
columns	A character string of the selected variable names. This field is a placeholder and will be populated once <code>prep()</code> is used.
keep_original_cols	A logical to keep the original variables in the output. Defaults to FALSE.
skip	A logical. Should the step be skipped when the recipe is baked by <code>bake()</code> ? While all operations are baked when <code>prep()</code> is run, some operations may not be able to be conducted on new data (e.g. processing the outcome variable(s)). Care should be taken when using <code>skip = TRUE</code> as it may affect the computations for subsequent operations.
id	A character string that is unique to this step to identify it.

Details

Persistent homology is usually encoded as birth–death pairs (barcodes or diagrams), but the space of persistence data sets does not satisfy convenient statistical properties. Such applications as hypothesis testing and machine learning benefit from transformations of persistence data, often to Hilbert spaces (vector spaces with inner products and induced metrics).

Value

An updated version of recipe with the new step added to the sequence of any existing operations.

Engine

The persistence silhouette vectorization deploys `TDavec::computePersistenceSilhouette()`. See there for definitions and references.

Tuning Parameters

This step has 2 tuning parameters:

- `hom_degree`: Homological degree (type: integer, default: 0L)
- `weight_power`: Exponent weight (type: double, default: 1)

Examples

```
library(recipes)

# inspect vectorized features
volc_dat <- data.frame(image = I(list(volcano / 10)))
recipe(~ image, data = volc_dat) %>%
  step_pd_raster(image, method = "link_join") %>%
  step_vpd_persistence_silhouette(image, hom_degree = 1) %>%
  print() -> volc_rec
```

```

print(volc_rec)
volc_rec %>%
  prep(training = volc_dat) %>%
  bake(new_data = volc_dat)

# dimension-reduce using vectorized features
data(permeability_qsar, package = "modeldata")
permeability_qsar %>%
  transform(perm_cut = cut(permeability, breaks = seq(0, 60, 10))) %>%
  subset(select = -permeability) %>%
  tidyr::nest(chem_fp = -perm_cut) %>%
  print() -> perm_dat
recipe(perm_cut ~ chem_fp, data = perm_dat) %>%
  step_pd_point_cloud(chem_fp, max_hom_degree = 2) %>%
  step_vpd_persistence_silhouette(chem_fp, hom_degree = 1) %>%
  step_pca(starts_with("chem_fp_"), num_comp = 2) %>%
  print() -> perm_rec
perm_est <- prep(perm_rec, training = perm_dat)
perm_res <- bake(perm_est, new_data = perm_dat)
# inspect results
tidy(perm_rec)
tidy(perm_rec, number = 2)
tidy(perm_est, number = 2)
# visualize results
with(perm_res, {
  plot(PC1, PC2, type = "n", asp = 1)
  text(PC1, PC2, labels = perm_cut)
})

```

```
step_vpd_persistent_entropy_summary
```

Persistent Entropy Summary Vectorization of Persistent Homology

Description

The function `step_vpd_persistent_entropy_summary()` creates a *specification* of a recipe step that will convert a list-column of 3-column matrices of persistence data to a list-column of 1-row matrices of vectorizations.

Usage

```

step_vpd_persistent_entropy_summary(
  recipe,
  ...,
  role = "predictor",
  trained = FALSE,
  hom_degree = 0L,
  xseq = NULL,
  xmin = NULL,

```

```

xmax = NULL,
xlen = NULL,
xby = NULL,
evaluate = "intervals",
columns = NULL,
keep_original_cols = TRUE,
skip = FALSE,
id = rand_id("vpd_persistent_entropy_summary")
)

```

Arguments

recipe	A recipe object. The step will be added to the sequence of operations for this recipe.
...	One or more selector functions to choose variables for this step. See selections() for more details.
role	For model terms created by this step, what analysis role should they be assigned? By default, the new columns created by this step from the original variables will be used as <i>predictors</i> in a model.
trained	A logical to indicate if the quantities for preprocessing have been estimated.
hom_degree	The homological degree of the features to be transformed.
xseq	A discretization grid, as an increasing numeric vector. xseq overrides the other x* parameters with a warning.
xmin, xmax, xlen, xby	Limits and resolution of a discretization grid; specify only one of xlen and xby.
evaluate	The method by which to vectorize continuous functions over a grid, either 'intervals' or 'points'. Some functions only admit one method.
columns	A character string of the selected variable names. This field is a placeholder and will be populated once prep() is used.
keep_original_cols	A logical to keep the original variables in the output. Defaults to FALSE.
skip	A logical. Should the step be skipped when the recipe is baked by bake() ? While all operations are baked when prep() is run, some operations may not be able to be conducted on new data (e.g. processing the outcome variable(s)). Care should be taken when using skip = TRUE as it may affect the computations for subsequent operations.
id	A character string that is unique to this step to identify it.

Details

Persistent homology is usually encoded as birth–death pairs (barcodes or diagrams), but the space of persistence data sets does not satisfy convenient statistical properties. Such applications as hypothesis testing and machine learning benefit from transformations of persistence data, often to Hilbert spaces (vector spaces with inner products and induced metrics).

Value

An updated version of recipe with the new step added to the sequence of any existing operations.

Engine

The persistent entropy summary vectorization deploys `TDAvec::computePersistentEntropy()`. See there for definitions and references.

Tuning Parameters

This step has 1 tuning parameter:

- `hom_degree`: Homological degree (type: integer, default: 0L)

Examples

```
library(recipes)

# inspect vectorized features
volc_dat <- data.frame(image = I(list(volcano / 10)))
recipe(~ image, data = volc_dat) %>%
  step_pd_raster(image, method = "link_join") %>%
  step_vpd_persistent_entropy_summary(image, hom_degree = 1) %>%
  print() -> volc_rec
print(volc_rec)
volc_rec %>%
  prep(training = volc_dat) %>%
  bake(new_data = volc_dat)

# dimension-reduce using vectorized features
data(permeability_qsar, package = "modeldata")
permeability_qsar %>%
  transform(perm_cut = cut(permeability, breaks = seq(0, 60, 10))) %>%
  subset(select = -permeability) %>%
  tidyr::nest(chem_fp = -perm_cut) %>%
  print() -> perm_dat
recipe(perm_cut ~ chem_fp, data = perm_dat) %>%
  step_pd_point_cloud(chem_fp, max_hom_degree = 2) %>%
  step_vpd_persistent_entropy_summary(chem_fp, hom_degree = 1) %>%
  step_pca(starts_with("chem_fp"), num_comp = 2) %>%
  print() -> perm_rec
perm_est <- prep(perm_rec, training = perm_dat)
perm_res <- bake(perm_est, new_data = perm_dat)
# inspect results
tidy(perm_rec)
tidy(perm_rec, number = 2)
tidy(perm_est, number = 2)
# visualize results
with(perm_res, {
  plot(PC1, PC2, type = "n", asp = 1)
  text(PC1, PC2, labels = perm_cut)
})
```

 step_vpd_tent_template_functions

Tent Template Functions Vectorization of Persistent Homology

Description

The function `step_vpd_tent_template_functions()` creates a *specification* of a recipe step that will convert a list-column of 3-column matrices of persistence data to a list-column of 1-row matrices of vectorizations.

Usage

```
step_vpd_tent_template_functions(
  recipe,
  ...,
  role = "predictor",
  trained = FALSE,
  hom_degree = 0L,
  tent_size = NULL,
  num_bins = 10L,
  tent_shift = NULL,
  columns = NULL,
  keep_original_cols = TRUE,
  skip = FALSE,
  id = rand_id("vpd_tent_template_functions")
)
```

Arguments

<code>recipe</code>	A recipe object. The step will be added to the sequence of operations for this recipe.
<code>...</code>	One or more selector functions to choose variables for this step. See selections() for more details.
<code>role</code>	For model terms created by this step, what analysis role should they be assigned? By default, the new columns created by this step from the original variables will be used as <i>predictors</i> in a model.
<code>trained</code>	A logical to indicate if the quantities for preprocessing have been estimated.
<code>hom_degree</code>	The homological degree of the features to be transformed.
<code>tent_size</code>	The length of the increment used to discretize tent template functions.
<code>num_bins</code>	The number of bins along each axis in the discretization grid.
<code>tent_shift</code>	The vertical shift applied to the discretization grid.
<code>columns</code>	A character string of the selected variable names. This field is a placeholder and will be populated once prep() is used.
<code>keep_original_cols</code>	A logical to keep the original variables in the output. Defaults to FALSE.

skip	A logical. Should the step be skipped when the recipe is baked by <code>bake()</code> ? While all operations are baked when <code>prep()</code> is run, some operations may not be able to be conducted on new data (e.g. processing the outcome variable(s)). Care should be taken when using <code>skip = TRUE</code> as it may affect the computations for subsequent operations.
id	A character string that is unique to this step to identify it.

Details

Persistent homology is usually encoded as birth–death pairs (barcodes or diagrams), but the space of persistence data sets does not satisfy convenient statistical properties. Such applications as hypothesis testing and machine learning benefit from transformations of persistence data, often to Hilbert spaces (vector spaces with inner products and induced metrics).

Value

An updated version of recipe with the new step added to the sequence of any existing operations.

Engine

The tent template functions vectorization deploys `TDavec::computeTemplateFunction()`. See there for definitions and references.

Tuning Parameters

This step has 4 tuning parameters:

- `hom_degree`: Homological degree (type: integer, default: 0L)
- `tent_size`: Discretization grid increment (type: double, default: NULL)
- `num_bins`: Discretization grid bins (type: integer, default: 10L)
- `tent_shift`: Discretization grid shift (type: double, default: NULL)

Examples

```
library(recipes)

# inspect vectorized features
volc_dat <- data.frame(image = I(list(volcano / 10)))
recipe(~ image, data = volc_dat) %>%
  step_pd_raster(image, method = "link_join") %>%
  step_vpd_tent_template_functions(image, hom_degree = 1) %>%
  print() -> volc_rec
print(volc_rec)
volc_rec %>%
  prep(training = volc_dat) %>%
  bake(new_data = volc_dat)

# dimension-reduce using vectorized features
data(permeability_qsar, package = "modeldata")
permeability_qsar %>%
```

```

transform(perm_cut = cut(permeability, breaks = seq(0, 60, 10))) %>%
subset(select = -permeability) %>%
tidyr::nest(chem_fp = -perm_cut) %>%
print() -> perm_dat
recipe(perm_cut ~ chem_fp, data = perm_dat) %>%
  step_pd_point_cloud(chem_fp, max_hom_degree = 2) %>%
  step_vpd_tent_template_functions(chem_fp, hom_degree = 1) %>%
  step_pca(starts_with("chem_fp_"), num_comp = 2) %>%
  print() -> perm_rec
perm_est <- prep(perm_rec, training = perm_dat)
perm_res <- bake(perm_est, new_data = perm_dat)
# inspect results
tidy(perm_rec)
tidy(perm_rec, number = 2)
tidy(perm_est, number = 2)
# visualize results
with(perm_res, {
  plot(PC1, PC2, type = "n", asp = 1)
  text(PC1, PC2, labels = perm_cut)
})

```

step_vpd_tropical_coordinates

Tropical Coordinates Vectorization of Persistent Homology

Description

The function `step_vpd_tropical_coordinates()` creates a *specification* of a recipe step that will convert a list-column of 3-column matrices of persistence data to a list-column of 1-row matrices of vectorizations.

Usage

```

step_vpd_tropical_coordinates(
  recipe,
  ...,
  role = "predictor",
  trained = FALSE,
  hom_degree = 0L,
  num_bars = 1L,
  columns = NULL,
  keep_original_cols = TRUE,
  skip = FALSE,
  id = rand_id("vpd_tropical_coordinates")
)

```

Arguments

recipe	A recipe object. The step will be added to the sequence of operations for this recipe.
...	One or more selector functions to choose variables for this step. See selections() for more details.
role	For model terms created by this step, what analysis role should they be assigned? By default, the new columns created by this step from the original variables will be used as <i>predictors</i> in a model.
trained	A logical to indicate if the quantities for preprocessing have been estimated.
hom_degree	The homological degree of the features to be transformed.
num_bars	Number of bars (persistent pairs) over which to maximize....
columns	A character string of the selected variable names. This field is a placeholder and will be populated once prep() is used.
keep_original_cols	A logical to keep the original variables in the output. Defaults to FALSE.
skip	A logical. Should the step be skipped when the recipe is baked by bake() ? While all operations are baked when prep() is run, some operations may not be able to be conducted on new data (e.g. processing the outcome variable(s)). Care should be taken when using <code>skip = TRUE</code> as it may affect the computations for subsequent operations.
id	A character string that is unique to this step to identify it.

Details

Persistent homology is usually encoded as birth–death pairs (barcodes or diagrams), but the space of persistence data sets does not satisfy convenient statistical properties. Such applications as hypothesis testing and machine learning benefit from transformations of persistence data, often to Hilbert spaces (vector spaces with inner products and induced metrics).

Value

An updated version of recipe with the new step added to the sequence of any existing operations.

Engine

The tropical coordinates vectorization deploys `TDAvec::computeTropicalCoordinates()`. See there for definitions and references.

Tuning Parameters

This step has 2 tuning parameters:

- `hom_degree`: Homological degree (type: integer, default: 0L)
- `num_bars`: # Bars (persistence pairs) (type: integer, default: 1L)

Examples

```

library(recipes)

# inspect vectorized features
volc_dat <- data.frame(image = I(list(volcano / 10)))
recipe(~ image, data = volc_dat) %>%
  step_pd_raster(image, method = "link_join") %>%
  step_vpd_tropical_coordinates(image, hom_degree = 1) %>%
  print() -> volc_rec
print(volc_rec)
volc_rec %>%
  prep(training = volc_dat) %>%
  bake(new_data = volc_dat)

# dimension-reduce using vectorized features
data(permeability_qsar, package = "modeldata")
permeability_qsar %>%
  transform(perm_cut = cut(permeability, breaks = seq(0, 60, 10))) %>%
  subset(select = -permeability) %>%
  tidyr::nest(chem_fp = -perm_cut) %>%
  print() -> perm_dat
recipe(perm_cut ~ chem_fp, data = perm_dat) %>%
  step_pd_point_cloud(chem_fp, max_hom_degree = 2) %>%
  step_vpd_tropical_coordinates(chem_fp, hom_degree = 1) %>%
  step_pca(starts_with("chem_fp_"), num_comp = 2) %>%
  print() -> perm_rec
perm_est <- prep(perm_rec, training = perm_dat)
perm_res <- bake(perm_est, new_data = perm_dat)
# inspect results
tidy(perm_rec)
tidy(perm_rec, number = 2)
tidy(perm_est, number = 2)
# visualize results
with(perm_res, {
  plot(PC1, PC2, type = "n", asp = 1)
  text(PC1, PC2, labels = perm_cut)
})

```

Description

These tuning functions govern the parameters of vectorizations implemented in **TDAvec**.

Usage

```
num_coef(range = c(1L, unknown()), trans = NULL)
```

```

poly_type(values = c("R", "S", "T"), trans = NULL)

img_sigma(range = c(unknown(), unknown()), trans = transform_log10())

num_levels(range = c(1L, unknown()), trans = NULL)

weight_func_pl(
  values = c("triangle", "epanechnikov", "tricubic"),
  trans = NULL
)

bandwidth(range = c(unknown(), unknown()), trans = transform_log10())

weight_power(range = c(1, 2), trans = NULL)

num_bars(range = c(1L, unknown()), trans = NULL)

num_bins(range = c(2L, 20L), trans = NULL)

tent_shift(range = c(unknown(), unknown()), trans = transform_log10())

```

Arguments

range	A two-element vector holding the <i>defaults</i> for the smallest and largest possible values, respectively. If a transformation is specified, these values should be in the <i>transformed units</i> .
trans	A trans object from the scales package, such as <code>scales::transform_log10()</code> or <code>scales::transform_reciprocal()</code> . If not provided, the default is used which matches the units used in range. If no transformation, NULL.
values	A character string of possible values.

Details

The parameter `num_coef` is passed to `m` in `TDAvec::computeComplexPolynomial()`.

The parameter `poly_type` is passed to `polyType` in `TDAvec::computeComplexPolynomial()`.

The parameter `img_sigma` is passed to `sigma` in `TDAvec::computePersistenceImage()`.

The parameter `num_levels` is passed to `k` in `TDAvec::computePersistenceLandscape()`.

The parameter `weight_func_pl` is passed to `kernel` in `TDAvec::computePersistenceLandscape()`.

The parameter `bandwidth` is passed to `h` in `TDAvec::computePersistenceLandscape()`.

The parameter `weight_power` is passed to `p` in `TDAvec::computePersistenceSilhouette()`.

The parameter `num_bars` is passed to `r` in `TDAvec::computeTropicalCoordinates()`.

The parameter `num_bins` is passed to `d` in `TDAvec::computeTemplateFunction()`.

The parameter `tent_shift` is passed to `epsilon` in `TDAvec::computeTemplateFunction()`.

Value

A param object or list of param objects.

Examples

```
data.frame(dist = I(list(eurodist, UScitiesD * 1.6))) %>%
  transform(pd = I(lapply(dist, ripserr::vietoris_rips))) %>%
  subset(select = c(pd)) %>%
  print() -> pd_data

# `num_coef` for `step_vpn_complex_polynomial()`

(nc_man <- num_coef(range = c(1L, 3L)))
grid_regular(nc_man)

# `poly_type` for `step_vpn_complex_polynomial()`

(pt_man <- poly_type(values = c("R", "S")))
grid_regular(pt_man)

# `img_sigma` for `step_vpn_persistence_image()`

(is_man <- img_sigma(range = c(100, 400), trans = NULL))
grid_regular(is_man)

(is_dat <- img_sigma() %>% get_pers_max_frac(x = pd_data))
grid_regular(is_dat)

(is_hom <- img_sigma() %>% get_pers_max_frac(x = pd_data, hom_degrees = seq(2L)))
grid_regular(is_hom)

# `num_levels` for `step_vpn_persistence_landscape()`

(nl_man <- num_levels(range = c(1L, 6L)))
grid_regular(nl_man)

# `weight_func_pl` for `step_vpn_persistence_landscape()`

(wfp_man <- weight_func_pl(values = c("triangle", "tricubic")))
grid_regular(wfp_man)

# `bandwidth` for `step_vpn_persistence_landscape()`

(b_man <- bandwidth(range = c(500, 1500), trans = NULL))
grid_regular(b_man)

(b_dat <- bandwidth() %>% get_pers_max_frac(x = pd_data))
grid_regular(b_dat)

(b_hom <- bandwidth() %>% get_pers_max_frac(x = pd_data, hom_degrees = seq(2L)))
grid_regular(b_hom)
```

```

# `weight_power` for `step_vpn_persistence_silhouette()`

(wp_man <- weight_power(range = c(1, 3)))
grid_regular(wp_man)

# `num_bars` for `step_vpn_tropical_coordinates()`

(nb_man <- num_bars(range = c(1L, 3L)))
grid_regular(nb_man)

# `num_bins` for `step_vpn_tent_template_functions()`

(nb_man <- num_bins(range = c(5L, 10L)))
grid_regular(nb_man)

# `tent_shift` for `step_vpn_tent_template_functions()`

(ts_man <- tent_shift(range = c(100, 200), trans = NULL))
grid_regular(ts_man)

(ts_dat <- tent_shift() %>% get_pers_min_mult(x = pd_data))
grid_regular(ts_dat)

(ts_hom <- tent_shift() %>% get_pers_min_mult(x = pd_data, hom_degrees = seq(2L)))
grid_regular(ts_hom)

```

vpd-finalizers

Finalizers for persistent homology vectorizations

Description

These functions take a persistent homology vectorization parameter object and modify the `dials::unknown()` parts of ranges based on a data set and heuristics used in inaugural studies.

Usage

```

get_pairs_max(object, x, hom_degrees = NULL, ...)

get_pers_max_frac(
  object,
  x,
  hom_degree = NULL,
  log_vals = TRUE,
  frac = 1/100,
  ...
)

get_pers_min_mult(

```

```

    object,
    x,
    hom_degree = NULL,
    log_vals = TRUE,
    mult = 100,
    ...
)

```

Arguments

<code>object</code>	A param object or a list of param objects.
<code>x</code>	Persistence data in a recognizable format.
<code>...</code>	Other arguments to pass to the underlying parameter finalizer functions.
<code>hom_degree, hom_degrees</code>	Integer (vector) of homological degree(s).
<code>log_vals</code>	A logical: should the ranges be set on the log10 scale?
<code>frac</code>	A double for the fraction of the data to be used for the upper bound. For <code>get_n_frac_range()</code> and <code>get_batch_sizes()</code> , a vector of two fractional values are required.
<code>mult</code>	A double for the multiple of the data to be used for the lower bound.

Details

`get_pairs_max()` sets the upper bound to the maximum number of persistent pairs.

`get_pers_max_frac()` sets both bounds to fractions of the maximum finite persistence (lifespan). A single number is used as the lower bound fraction and takes the upper bound fraction to be 1.

`get_pers_min_mult()` sets both bounds to multiples of the minimum positive persistence (lifespan). A single number is used as the upper bound multiple and takes the lower bound multiple to be 1.

Value

An updated param object or a list of updated param objects depending on what is provided in `object`.

vpd-summarizers

Summarize topological data

Description

These miscellaneous functions are used by various `get_*_range()` functions to [finalize](#) hyperparameter ranges.

Usage

```
ph_dim(x)

## Default S3 method:
ph_dim(x)

## S3 method for class 'matrix'
ph_dim(x)

## S3 method for class 'array'
ph_dim(x)

## S3 method for class 'data.frame'
ph_dim(x)

## S3 method for class 'dist'
ph_dim(x)

## S3 method for class 'ts'
ph_dim(x)

pairs_min(x, hom_degrees)

## Default S3 method:
pairs_min(x, hom_degrees)

## S3 method for class 'matrix'
pairs_min(x, hom_degrees)

## S3 method for class 'data.frame'
pairs_min(x, hom_degrees)

## S3 method for class 'diagram'
pairs_min(x, hom_degrees)

## S3 method for class 'PHom'
pairs_min(x, hom_degrees)

## S3 method for class 'persistence'
pairs_min(x, hom_degrees)

pairs_max(x, hom_degrees)

## Default S3 method:
pairs_max(x, hom_degrees)

## S3 method for class 'matrix'
pairs_max(x, hom_degrees)
```

```
## S3 method for class 'data.frame'
pairs_max(x, hom_degrees)

## S3 method for class 'diagram'
pairs_max(x, hom_degrees)

## S3 method for class 'PHom'
pairs_max(x, hom_degrees)

## S3 method for class 'persistence'
pairs_max(x, hom_degrees)

birth_range(x, hom_degree)

## Default S3 method:
birth_range(x, hom_degree)

## S3 method for class 'matrix'
birth_range(x, hom_degree)

## S3 method for class 'data.frame'
birth_range(x, hom_degree)

## S3 method for class 'diagram'
birth_range(x, hom_degree)

## S3 method for class 'PHom'
birth_range(x, hom_degree)

## S3 method for class 'persistence'
birth_range(x, hom_degree)

pers_max(x, hom_degree)

## Default S3 method:
pers_max(x, hom_degree)

## S3 method for class 'matrix'
pers_max(x, hom_degree)

## S3 method for class 'data.frame'
pers_max(x, hom_degree)

## S3 method for class 'diagram'
pers_max(x, hom_degree)

## S3 method for class 'PHom'
```

```
pers_max(x, hom_degree)

## S3 method for class 'persistence'
pers_max(x, hom_degree)

pers_min(x, hom_degree)

## Default S3 method:
pers_min(x, hom_degree)

## S3 method for class 'matrix'
pers_min(x, hom_degree)

## S3 method for class 'data.frame'
pers_min(x, hom_degree)

## S3 method for class 'diagram'
pers_min(x, hom_degree)

## S3 method for class 'PHom'
pers_min(x, hom_degree)

## S3 method for class 'persistence'
pers_min(x, hom_degree)

pers_range(x, hom_degree)

## Default S3 method:
pers_range(x, hom_degree)

## S3 method for class 'matrix'
pers_range(x, hom_degree)

## S3 method for class 'data.frame'
pers_range(x, hom_degree)

## S3 method for class 'diagram'
pers_range(x, hom_degree)

## S3 method for class 'PHom'
pers_range(x, hom_degree)

## S3 method for class 'persistence'
pers_range(x, hom_degree)

life_support(x, hom_degree)

## Default S3 method:
```

```
life_support(x, hom_degree)

## S3 method for class 'matrix'
life_support(x, hom_degree)

## S3 method for class 'data.frame'
life_support(x, hom_degree)

## S3 method for class 'diagram'
life_support(x, hom_degree)

## S3 method for class 'PHom'
life_support(x, hom_degree)

## S3 method for class 'persistence'
life_support(x, hom_degree)
```

Arguments

`x` Persistence data in a recognizable format.
`hom_degree, hom_degrees` Integer (vector) of homological degree(s).

Details

The functions compute the following summaries:

- `ph_dim()`: Dimension of a data set for purposes of PH
- `pairs_min()`: Minimum number of persistent pairs of any degree
- `pairs_max()`: Maximum number of persistent pairs of any degree
- `birth_range()`: Range of finite birth values for a given degree
- `pers_max()`: Maximum positive finite persistence for a given degree
- `pers_min()`: Minimum positive finite persistence for a given degree
- `pers_range()`: Range of positive finite persistence for a given degree
- `life_support()`: Range of union of birth–death ranges for a given degree

Value

A vector of one or two numeric values.

Index

- * **datasets**
 - mnist, [6](#)
- * **topological feature extraction via persistent homology**
 - step_pd_degree, [8](#)
 - step_pd_point_cloud, [10](#)
 - step_pd_raster, [12](#)
- bake(), [7](#), [9](#), [11](#), [13](#), [15](#), [18](#), [20](#), [22](#), [25](#), [27](#), [30](#), [32](#), [35](#), [38](#), [40](#), [43](#), [45](#)
- bandwidth (vpd-dials), [46](#)
- birth_range (vpd-summarizers), [50](#)
- blur, [2](#)
- blur(), [4](#), [7](#)
- blur_sigmas, [4](#)
- dials::unknown(), [49](#)
- finalize, [50](#)
- get_blur_range, [5](#)
- get_hom_range (get_blur_range), [5](#)
- get_pairs_max (vpd-finalizers), [49](#)
- get_pers_max_frac (vpd-finalizers), [49](#)
- get_pers_min_mult (vpd-finalizers), [49](#)
- hom_degree (get_blur_range), [5](#)
- img_sigma (vpd-dials), [46](#)
- kernlab::sigest(), [5](#)
- life_support (vpd-summarizers), [50](#)
- max_hom_degree (get_blur_range), [5](#)
- mnist, [6](#)
- mnist_test (mnist), [6](#)
- mnist_train (mnist), [6](#)
- num_bars (vpd-dials), [46](#)
- num_bins (vpd-dials), [46](#)
- num_coef (vpd-dials), [46](#)
- num_levels (vpd-dials), [46](#)
- pairs_max (vpd-summarizers), [50](#)
- pairs_min (vpd-summarizers), [50](#)
- pers_max (vpd-summarizers), [50](#)
- pers_min (vpd-summarizers), [50](#)
- pers_range (vpd-summarizers), [50](#)
- ph_dim (vpd-summarizers), [50](#)
- poly_type (vpd-dials), [46](#)
- prep(), [7](#), [9](#), [11](#), [13](#), [15](#), [18](#), [20](#), [22](#), [25](#), [27](#), [30](#), [32](#), [35](#), [38](#), [40](#), [42](#), [43](#), [45](#)
- ripserr, [11](#), [14](#)
- selections(), [7](#), [9](#), [10](#), [13](#), [15](#), [17](#), [20](#), [22](#), [24](#), [27](#), [29](#), [32](#), [35](#), [37](#), [40](#), [42](#), [45](#)
- step_blur, [7](#)
- step_pd_degree, [8](#), [12](#), [14](#)
- step_pd_point_cloud, [9](#), [10](#), [14](#)
- step_pd_raster, [9](#), [12](#), [12](#)
- step_vpd_algebraic_functions, [14](#)
- step_vpd_betti_curve, [17](#)
- step_vpd_complex_polynomial, [19](#)
- step_vpd_descriptive_statistics, [21](#)
- step_vpd_euler_characteristic_curve, [24](#)
- step_vpd_normalized_life_curve, [26](#)
- step_vpd_persistence_block, [28](#)
- step_vpd_persistence_image, [31](#)
- step_vpd_persistence_landscape, [34](#)
- step_vpd_persistence_silhouette, [37](#)
- step_vpd_persistent_entropy_summary, [39](#)
- step_vpd_tent_template_functions, [42](#)
- step_vpd_tropical_coordinates, [44](#)
- TDA, [11](#)
- TDAvec::computeAlgebraicFunctions(), [16](#)

- TDavec::computeBettiCurve(), [18](#)
- TDavec::computeComplexPolynomial(), [20](#), [47](#)
- TDavec::computeEulerCharacteristic(), [25](#)
- TDavec::computeNormalizedLife(), [27](#)
- TDavec::computePersistenceBlock(), [30](#)
- TDavec::computePersistenceImage(), [33](#), [47](#)
- TDavec::computePersistenceLandscape(), [35](#), [47](#)
- TDavec::computePersistenceSilhouette(), [38](#), [47](#)
- TDavec::computePersistentEntropy(), [41](#)
- TDavec::computeStats(), [23](#)
- TDavec::computeTemplateFunction(), [43](#), [47](#)
- TDavec::computeTropicalCoordinates(), [45](#), [47](#)
- tent_shift (vpd-dials), [46](#)
- tidy.step_blur (step_blur), [7](#)
- tidy.step_pd_degree (step_pd_degree), [8](#)
- tidy.step_pd_point_cloud (step_pd_point_cloud), [10](#)
- tidy.step_pd_raster (step_pd_raster), [12](#)
- tidy.step_vpd_algebraic_functions (step_vpd_algebraic_functions), [14](#)
- tidy.step_vpd_betti_curve (step_vpd_betti_curve), [17](#)
- tidy.step_vpd_complex_polynomial (step_vpd_complex_polynomial), [19](#)
- tidy.step_vpd_descriptive_statistics (step_vpd_descriptive_statistics), [21](#)
- tidy.step_vpd_euler_characteristic_curve (step_vpd_euler_characteristic_curve), [24](#)
- tidy.step_vpd_normalized_life_curve (step_vpd_normalized_life_curve), [26](#)
- tidy.step_vpd_persistence_block (step_vpd_persistence_block), [28](#)
- tidy.step_vpd_persistence_image (step_vpd_persistence_image), [31](#)
- tidy.step_vpd_persistence_landscape (step_vpd_persistence_landscape), [34](#)
- tidy.step_vpd_persistence_silhouette (step_vpd_persistence_silhouette), [37](#)
- tidy.step_vpd_persistent_entropy_summary (step_vpd_persistent_entropy_summary), [39](#)
- tidy.step_vpd_tent_template_functions (step_vpd_tent_template_functions), [42](#)
- tidy.step_vpd_tropical_coordinates (step_vpd_tropical_coordinates), [44](#)
- vpd-dials, [46](#)
- vpd-finalizers, [49](#)
- vpd-summarizers, [50](#)
- weight_func_pl (vpd-dials), [46](#)
- weight_power (vpd-dials), [46](#)