

Package ‘destiny’

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Type Package

Title Creates diffusion maps

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Description Create and plot diffusion maps.

License GPL

URL <https://github.com/theislab/destiny>

BugReports <https://github.com/theislab/destiny/issues>

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Depends R (>= 3.3.0)

Imports methods, graphics, grDevices, utils, stats, Matrix, Rcpp (>= 0.10.3), RcppEigen, Biobase, BiocGenerics, SummarizedExperiment, ggplot2, ggthemes, VIM, proxy, igraph, smoother, scales, scatterplot3d

LinkingTo Rcpp, RcppEigen, grDevices

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VignetteBuilder nbconvertR

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Collate 'RcppExports.R' 'aaa.r' 'accessor-generics.r' 'censoring.r' 'colorlegend.r' 'compat.r' 'cube_helix.r' 'dataset-helpers.r' 'destiny-package.r' 's4-unions.r' 'dist-matrix-coerce.r' 'sigmas.r' 'diffusionmap.r' 'diffusionmap-methods-accession.r' 'diffusionmap-methods.r' 'plohelpers.r' 'diffusionmap-plotting.r' 'dpt-branching.r' 'dpt-helpers.r' 'dpt.r' 'dpt-methods-matrix.r' 'dpt-methods.r' 'utils.r' 'dpt-plotting.r' 'eig_decomp.r' 'expressionset-helpers.r' 'find_dm_k.r' 'gene-relevance.r' 'gene-relevance-methods.r' 'gene-relevance-plotting.r' 'guo-data.r' 'knn.r' 'l_which.r' 'methods-coercion.r' 'methods-extraction.r' 'methods-update.r' 'predict.r' 'projection-dist.r' 'rankcor.r' 'sigmas-plotting.r'

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coercions

Coercion methods

Description

Convert a [DiffusionMap](#) or [DPT](#) object to other classes

Usage

```
## S4 method for signature 'DiffusionMap'  
as.data.frame(x, row.names = NULL,  
  optional = FALSE, ...)  
  
fortify.DiffusionMap(model, data, ...)  
  
## S4 method for signature 'DPT'  
as.data.frame(x, row.names = NULL, optional = FALSE, ...)  
  
fortify.DPT(model, data, ...)  
  
## S4 method for signature 'DPT'  
as.matrix(x, ...)
```

Arguments

<code>x, model</code>	A DiffusionMap or DPT object
<code>row.names</code>	NULL or a character vector giving the row names for the data frame. Missing values are not allowed.
<code>optional</code>	logical. If TRUE, setting row names and converting column names (to syntactic names: see <code>make.names</code>) is optional.
<code>...</code>	Passed to as.data.frame
<code>data</code>	ignored

Details

[fortify](#) is a `ggplot2` generic allowing a diffusion map to be used as data parameter in [ggplot](#) or [qplot](#).

Value

An object of the desired class

See Also

[DiffusionMap accessors, extractions, DiffusionMap methods](#) for more methods

Examples

```

library(Biobase)
data(guo)
dm <- DiffusionMap(guo)
classes <- vapply(as.data.frame(dm), class, character(1L))
stopifnot(all(classes[paste0('DC', 1:20)] == 'numeric'))
stopifnot(all(classes[featureNames(guo) ] == 'numeric'))
stopifnot(all(classes[ varLabels(guo) ] == c('factor', 'integer')))

```

colorlegend

*Color legend***Description**

Creates a color legend for a vector used to color a plot. It will use the current `palette()` or the specified `pal` as reference.

Usage

```

colorlegend(col, pal = palette(), log = FALSE, posx = c(0.9, 0.93),
  posy = c(0.05, 0.9), main = NULL, cex_main = par("cex.sub"),
  cex_axis = par("cex.axis"), col_main = par("col.sub"),
  col_lab = par("col.lab"), steps = 5, steps_color = 100, digit = 2,
  left = FALSE, ..., cex.main = NULL, cex.axis = NULL, col.main = NULL,
  col.lab = NULL)

```

Arguments

<code>col</code>	Vector of factor, integer, or double used to determine the ticks.
<code>pal</code>	If <code>col</code> is double, <code>pal</code> is used as a continuous palette, else as categorical one
<code>log</code>	Use logarithmic scale?
<code>posx</code>	Left and right borders of the color bar relative to plot area (Vector of length 2; 0-1)
<code>posy</code>	Bottom and top borders of color bar relative to plot area (Vector of length 2; 0-1)
<code>main</code>	Legend title
<code>cex_main</code>	Size of legend title font (default: subtitle font size <code>par('cex.sub')</code>)
<code>cex_axis</code>	Size of ticks/category labels (default: axis font size <code>par('cex.axis')</code>)
<code>col_main</code>	Color of legend title (default: subtitle color <code>par('col.sub')</code>)
<code>col_lab</code>	Color of tick or category labels (default: axis color <code>par('col.lab')</code>)
<code>steps</code>	Number of labels in case of a continuous axis. If 0 or FALSE, draw no ticks
<code>steps_color</code>	Number of gradient samples in case of continuous axis
<code>digit</code>	Number of digits for continuous axis labels
<code>left</code>	logical. If TRUE, invert <code>posx</code>
<code>...</code>	Additional parameters for the <code>text</code> call used for labels
<code>cex.main</code> , <code>cex.axis</code> , <code>col.main</code> , <code>col.lab</code>	For compatibility with <code>par</code>

Details

When passed a factor or integer vector, it will create a discrete legend, whereas a double vector will result in a continuous bar.

Value

This function is called for the side effect of adding a colorbar to a plot and returns nothing/NULL.

Examples

```
color_data <- 1:6
par(mar = par('mar') + c(0, 0, 0, 3))
plot(sample(6), col = color_data)
colorlegend(color_data)
```

 cube_helix

Sequential color palette using the cube helix system

Description

Creates a perceptually monotonously decreasing (or increasing) lightness color palette with different tones.

Usage

```
cube_helix(n = 6, start = 0, r = 0.4, hue = 0.8, gamma = 1,
  light = 0.85, dark = 0.15, reverse = FALSE)

scale_colour_cube_helix(..., start = 0, r = 0.4, hue = 0.8, gamma = 1,
  light = 0.85, dark = 0.15, reverse = FALSE, discrete = TRUE,
  guide = if (discrete) "legend" else "colourbar")

scale_color_cube_helix(..., start = 0, r = 0.4, hue = 0.8, gamma = 1,
  light = 0.85, dark = 0.15, reverse = FALSE, discrete = TRUE,
  guide = if (discrete) "legend" else "colourbar")

scale_fill_cube_helix(..., start = 0, r = 0.4, hue = 0.8, gamma = 1,
  light = 0.85, dark = 0.15, reverse = FALSE, discrete = TRUE,
  guide = if (discrete) "legend" else "colourbar")
```

Arguments

n	Number of colors to return (default: 6)
start	Hue to start helix at (start $\in [0, 3]$, default: 0)
r	Number of rotations of the helix. Can be negative. (default: 0.4)
hue	Saturation. 0 means greyscale, 1 fully saturated colors (default: 0.8)
gamma	Emphasize darker (gamma < 1) or lighter (gamma > 1) colors (default: 1)
light	Lightest lightness (default: 0.85)
dark	Darkest lightness (default: 0.15)

reverse	logical. If TRUE, reverse lightness (default: FALSE)
...	parameters passed to discrete_scale or continuous_scale
discrete	If TRUE, return a discrete scale, if FALSE a continuous one (default: TRUE)
guide	Type of scale guide to use. See guides

Value

A character vector of hex colors with length n

Examples

```
palette(cube_helix())
image(matrix(1:6), col = 1:6, pch = 19, axes = FALSE)

cr <- scales::colour_ramp(cube_helix(12, r = 3))
r <- runif(100)
plot(1:100, r, col = cr(r), type = 'b', pch = 20)
```

destiny	<i>Create and plot diffusion maps</i>
---------	---------------------------------------

Description

The main function is [DiffusionMap](#), which returns an object you can [plot](#) ([plot.DiffusionMap](#) is then called).

Examples

```
demo(destiny, ask = FALSE)
```

destiny generics	<i>destiny generics</i>
------------------	-------------------------

Description

destiny provides several generic methods and implements them for the [DiffusionMap](#) and [Sigmas](#) classes.

Usage

```
eigenvalues(object)

eigenvalues(object) <- value

eigenvectors(object)

eigenvectors(object) <- value
```

```
sigmas(object)
sigmas(object) <- value
dataset(object)
dataset(object) <- value
distance(object)
distance(object) <- value
optimal_sigma(object)
```

Arguments

object	Object from which to extract or to which to assign a value
value	Value to assign within an object

Value

eigenvalues retrieves the numeric eigenvalues
eigenvectors retrieves the eigenvectors matrix
sigmas retrieves the [Sigmas](#) from an object utilizing it as kernel width
dataset retrieves the data the object was created from
distance retrieves the distance metric used to create the object, e.g. euclidean
optimal_sigma retrieves the numeric value of the optimal sigma or local sigmas

See Also

[DiffusionMap methods](#) and [Sigmas class](#) for implementations

Examples

```
data(guo_norm)
dm <- DiffusionMap(guo_norm)
eigenvalues(dm)
eigenvectors(dm)
sigmas(dm)
optimal_sigma(dm)
dataset(dm)
distance(dm)
```

DiffusionMap accessors

DiffusionMap accession methods

Description

Get and set eigenvalues, eigenvectors, and sigma(s) of a [DiffusionMap](#) object or print information about a DiffusionMap

Usage

```
## S4 method for signature 'DiffusionMap'
eigenvalues(object)

## S4 replacement method for signature 'DiffusionMap'
eigenvalues(object) <- value

## S4 method for signature 'DiffusionMap'
eigenvectors(object)

## S4 replacement method for signature 'DiffusionMap'
eigenvectors(object) <- value

## S4 method for signature 'DiffusionMap'
sigmas(object)

## S4 replacement method for signature 'DiffusionMap'
sigmas(object) <- value

## S4 method for signature 'DiffusionMap'
dataset(object)

## S4 replacement method for signature 'DiffusionMap'
dataset(object) <- value

## S4 method for signature 'DiffusionMap'
distance(object)

## S4 replacement method for signature 'DiffusionMap'
distance(object) <- value

## S4 method for signature 'DiffusionMap'
optimal_sigma(object)
```

Arguments

object	A DiffusionMap
value	Vector of eigenvalues or matrix of eigenvectors to get/set

Value

The assigned or retrieved value

See Also

[extractions](#), [DiffusionMap methods](#), [coercions](#) for more methods

Examples

```
data(guo)
dm <- DiffusionMap(guo)
eigenvalues(dm)
eigenvectors(dm)
sigmas(dm)
dataset(dm)
optimal_sigma(dm)
```

DiffusionMap class *Create a diffusion map of cells*

Description

The provided data can be a double [matrix](#) of expression data or a [data.frame](#) with all non-integer (double) columns being treated as expression data features (and the others ignored), an [Expression-Set](#), or a [SingleCellExperiment](#).

Usage

```
DiffusionMap(data = stopifnot_distmatrix(distance), sigma = "local",
  k = find_dm_k(dataset_n_observations(data, distance) - 1L),
  n_eigs = min(20L, dataset_n_observations(data, distance) - 2L),
  density_norm = TRUE, ..., distance = c("euclidean", "cosine", "rankcor"),
  n_local = seq(to = min(k, 7L), length.out = min(k, 3L)), rotate = FALSE,
  censor_val = NULL, censor_range = NULL, missing_range = NULL,
  vars = NULL, verbose = !is.null(censor_range), suppress_dpt = FALSE)
```

Arguments

data	Expression data to be analyzed and covariates. Provide vars to select specific columns other than the default: all double value columns. If distance is a distance matrix, data has to be a data.frame with covariates only.
sigma	Diffusion scale parameter of the Gaussian kernel. One of 'local', 'global', a (numeric) global sigma or a Sigmas object. When choosing 'global', a global sigma will be calculated using find_sigmas . (Optional. default: 'local') A larger sigma might be necessary if the eigenvalues can not be found because of a singularity in the matrix
k	Number of nearest neighbors to consider (default: a guess between 100 and $n - 1$. See find_dm_k).
n_eigs	Number of eigenvectors/values to return (default: 20)
density_norm	logical. If TRUE, use density normalisation
...	Unused. All parameters to the right of the ... have to be specified by name (e.g. <code>DiffusionMap(data, distance = 'cosine')</code>)

distance	Distance measurement method applied to data or a distance matrix/ dist . For the allowed values, see find_knn
n_local	If <code>sigma == 'local'</code> , the <code>n_local</code> th nearest neighbor(s) determine(s) the local sigma
rotate	logical. If TRUE, rotate the eigenvalues to get a slimmer diffusion map
sensor_val	Value regarded as uncertain. Either a single value or one for every dimension (Optional, default: <code>sensor_val</code>)
sensor_range	Uncertainty range for censoring (Optional, default: none). A length-2-vector of certainty range start and end. TODO: also allow $2 \times G$ matrix
missing_range	Whole data range for missing value model. Has to be specified if NAs are in the data
vars	Variables (columns) of the data to use. Specifying NULL will select all columns (default: All floating point value columns)
verbose	Show a progressbar and other progress information (default: do it if censoring is enabled)
suppress_dpt	Specify TRUE to skip calculation of necessary (but spacious) information for DPT in the returned object (default: FALSE)

Value

A DiffusionMap object:

Slots

eigenvalues	Eigenvalues ranking the eigenvectors
eigenvectors	Eigenvectors mapping the datapoints to <code>n_eigs</code> dimensions
sigmas	Sigmas object with either information about the find_sigmas heuristic run or just local or optimal_sigma .
data_env	Environment referencing the data used to create the diffusion map
eigenvec0	First (constant) eigenvector not included as diffusion component.
transitions	Transition probabilities. Can be NULL
d	Density vector of transition probability matrix
d_norm	Density vector of normalized transition probability matrix
k	The <code>k</code> parameter for kNN
n_local	The <code>n_local</code> th nearest neighbor(s) is/are used to determine local kernel density
density_norm	Was density normalization used?
rotate	Were the eigenvectors rotated?
distance	Distance measurement method used
sensor_val	Censoring value
sensor_range	Censoring range
missing_range	Whole data range for missing value model
vars	Vars parameter used to extract the part of the data used for diffusion map creation

See Also

[DiffusionMap-methods](#) to get and set the slots. [find_sigmas](#) to pre-calculate a fitting global sigma parameter

Examples

```
data(guo)
DiffusionMap(guo)
DiffusionMap(guo, 13, censor_val = 15, censor_range = c(15, 40), verbose = TRUE)

covars <- data.frame(covar1 = letters[1:100])
dists <- dist(matrix(rnorm(100*10), 100))
DiffusionMap(covars, distance = dists)
```

DiffusionMap methods *DiffusionMap methods*

Description

Methods for external operations on diffusion maps

Usage

```
## S4 method for signature 'DiffusionMap'
print(x)

## S4 method for signature 'DiffusionMap'
show(object)
```

Arguments

x, object A [DiffusionMap](#)

Value

The DiffusionMap object (print), or NULL (show), invisibly

See Also

[DiffusionMap accessors, extractions, coercions](#) for more methods

Examples

```
data(guo)
dm <- DiffusionMap(guo)
print(dm)
show(dm)
```

dm_predict	<i>Predict new data points using an existing DiffusionMap. The resulting matrix can be used in the plot method for the DiffusionMap</i>
------------	---

Description

Predict new data points using an existing DiffusionMap. The resulting matrix can be used in [the plot method for the DiffusionMap](#)

Usage

```
dm_predict(dm, new_data, ..., verbose = FALSE)
```

Arguments

dm	A DiffusionMap object.
new_data	New data points to project into the diffusion map. Can be a matrix , data.frame , ExpressionSet , or SingleCellExperiment .
...	Passed to proxy::dist (new_data, data, dm@distance, ...).
verbose	Show progress messages?

Value

A $nrow(new_data) \times ncol(eigenvectors(dif))$ matrix of projected diffusion components for the new data.

Examples

```
data(guo)
g1 <- guo[, guo$num_cells != 32L]
g2 <- guo[, guo$num_cells == 32L]
dm <- DiffusionMap(g1)
dc2 <- dm_predict(dm, g2)
plot(dm, new_dcs = dc2)
```

DPT

Diffusion Pseudo Time

Description

Create pseudotime ordering and assigns cell to one of three branches

Usage

```
DPT(dm, tips = random_root(dm), ..., w_width = 0.1)
```

Arguments

dm	A <code>DiffusionMap</code> object. Its transition probabilities will be used to calculate the DPT
tips	The cell index/indices from which to calculate the DPT(s) (integer of length 1-3)
...	Unused. All parameters to the right of the ... have to be specified by name (e.g. <code>DPT(dm, w_width = 0.2)</code>)
w_width	Window width to use for deciding the branch cutoff

Details

Treat it as a matrix of pseudotime by subsetting (`[dim nrow ncol as.matrix)`), and as a list of pseudotime, and expression vectors (`$ [[names as.data.frame)`).

Value

A DPT object:

Slots

branch `matrix` (of `integer`) recursive branch labels for each cell (row); NA for undecided. Use `branch_divide` to modify this.

tips `matrix` (of `logical`) indicating if a cell (row) is a tip of the corresponding branch level (col)

dm `DiffusionMap` used to create this DPT object

Examples

```
data(guo_norm)
dm <- DiffusionMap(guo_norm)
dpt <- DPT(dm)
str(dpt)
```

DPT matrix methods *DPT Matrix methods*

Description

Treat DPT object as a matrix of cell-by-cell DPT distances.

Usage

```
## S4 method for signature 'DPT,index,index,logicalOrMissing'
x[i, j, ..., drop = TRUE]

## S4 method for signature 'DPT,index,missing,logicalOrMissing'
x[i, j, ..., drop = TRUE]

## S4 method for signature 'DPT,missing,index,logicalOrMissing'
x[i, j, ..., drop = TRUE]
```

```
## S4 method for signature 'DPT,missing,missing,logicalOrMissing'
x[i, j, ..., drop = TRUE]

## S4 method for signature 'DPT,index,index'
x[[i, j, ...]]

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

## S4 method for signature 'DPT'
ncol(x)

## S4 method for signature 'DPT'
dim(x)
```

Arguments

x	DPT object.
i, j	Numeric or logical index.
...	ignored
drop	If <code>TRUE</code> , coerce result to a vector if it would otherwise have <code>1 %in% dim(result)</code> .

See Also

[as.matrix.DPT](#)

DPT methods

DPT methods

Description

Methods for the [DPT](#) class. `branch_divide` subdivides branches for plotting (see the examples).

Usage

```
branch_divide(dpt, divide = integer(0L))

tips(dpt)

## S4 method for signature 'DPT'
dataset(object)

## S4 replacement method for signature 'DPT'
dataset(object) <- value
```

Arguments

dpt, object	DPT object
divide	Vector of branch numbers to use for division
value	Value of slot to set

Value

branch_divide and dataset<- return the changed object, dataset the extracted data, and tips the tip indices.

See Also

[plot.DPT](#) uses branch_divide for its divide argument.

Examples

```
data(guo_norm)
dpt <- DPT(DiffusionMap(guo_norm))
dpt_9_branches <- branch_divide(dpt, 1:3)
plot(dpt_9_branches, col_by = 'branch')
```

eig_decomp

Fast eigen decomposition using ARPACK

Description

Fast eigen decomposition using ARPACK

Usage

```
eig_decomp(M, n_eigs, sym = isSymmetric(M))
```

Arguments

M	A matrix (e.g. from the Matrix package)
n_eigs	Number of eigenvectors to return
sym	TRUE if M is symmetric

Value

n eigenvectors of the transition matrix

Examples

```
eig_decomp(cbind(c(1,-1), c(-1,1)), 2)
```

ExpressionSet helpers *Convert object to [ExpressionSet](#) or read it from a file*

Description

These functions present quick way to create [ExpressionSet](#) objects.

Usage

```
as.ExpressionSet(x, ...)

## S4 method for signature 'data.frame'
as.ExpressionSet(x, annotation_cols = !sapply(x,
  is.double))

read.ExpressionSet(file, header = TRUE, ...)
```

Arguments

x	data.frame to convert to an ExpressionSet .
...	Additional parameters to read.table
annotation_cols	The data.frame columns used as annotations. All others are used as expressions. (Logical, character or numerical index array)
file	File path to read ASCII data from
header	Specifies if the file has a header row.

Details

They work by using all continuous (double) columns as expression data, and all others as observation annotations.

Value

an [ExpressionSet](#) object

See Also

[read.table](#) on which `read.ExpressionSet` is based, and [ExpressionSet](#).

Examples

```
library(Biobase)
df <- data.frame(Time = seq_len(3), #integer column
  Actb = c(0.05, 0.3, 0.8),
  Gapdh = c(0.2, 0.03, 0.1))
set <- as.ExpressionSet(df)
rownames(exprs(set)) == c('Actb', 'Gapdh')
phenoData(set)$Time == 1:3
```

extractions *Extraction methods*

Description

Extraction methods

Usage

```
## S4 method for signature 'DiffusionMap'
names(x)

## S4 method for signature 'DPT'
names(x)

## S4 method for signature 'DiffusionMap,character,missing'
x[[i, j, ...]]

## S4 method for signature 'DPT,character,missing'
x[[i, j, ...]]

## S4 method for signature 'DiffusionMap'
x$name

## S4 method for signature 'DPT'
x$name
```

Arguments

x	DiffusionMap or DPT object
i, name	Name of a diffusion component 'DCx', 'DPTx', 'Branch' or column from the data
j	N/A
...	ignored

Value

The names or data row, see respective generics.

See Also

[Extract, names](#) for the generics. [DiffusionMap accessors](#), [DiffusionMap methods](#), [coercions](#) for more methods

Examples

```
data(guo)
dm <- DiffusionMap(guo)
dm$DC1        # A diffusion component
dm$Actb      # A gene expression vector
dm$num_cells # Phenotype metadata
```

```
dpt <- DPT(dm)
dm$Branch
dm$DPT1
```

find_dm_k	<i>Find a suitable k</i>
-----------	--------------------------

Description

The k parameter for the k nearest neighbors used in [DiffusionMap](#) should be as big as possible while still being computationally feasible. This function approximates it depending on the size of the dataset n .

Usage

```
find_dm_k(n, min_k = 100L, small = 1000L, big = 10000L)
```

Arguments

<code>n</code>	Number of possible neighbors (<code>nrow(dataset) - 1</code>)
<code>min_k</code>	Minimum number of neighbors. Will be chosen for $n \geq big$
<code>small</code>	Number of neighbors considered small. If/where $n \leq small$, n itself will be returned.
<code>big</code>	Number of neighbors considered big. If/where $n \geq big$, <code>min_k</code> will be returned.

Value

A vector of the same length as n that contains suitable k values for the respective n

Examples

```
curve(find_dm_k(n), 0, 13000, xname = 'n')
curve(find_dm_k(n) / n, 0, 13000, xname = 'n')
```

find_sigmas	<i>Calculate the average dimensionality for m different gaussian kernel widths (σ).</i>
-------------	--

Description

The sigma with the maximum value in average dimensionality is close to the ideal one. Increasing step number gets this nearer to the ideal one.

Usage

```
find_sigmas(data, step_size = 0.1, steps = 10L, start = NULL,
  sample_rows = 500L, early_exit = FALSE, ..., censor_val = NULL,
  censor_range = NULL, missing_range = NULL, vars = NULL,
  verbose = TRUE)
```

Arguments

data	Data set with n observations. Can be a data.frame , matrix , ExpressionSet or SingleCellExperiment .
step_size	Size of log-sigma steps
steps	Number of steps/calculations
start	Initial value to search from. (Optional. default: $\log_{10}(\min(\text{dist}(\text{data})))$)
sample_rows	Number of random rows to use for sigma estimation or vector of row indices/names to use. In the first case, only used if actually smaller than the number of available rows (Optional. default: 500)
early_exit	logical. If TRUE, return if the first local maximum is found, else keep running
...	Unused. All parameters to the right of the ... have to be specified by name (e.g. <code>find_sigmas(data, verbose = FALSE)</code>)
censor_val	Value regarded as uncertain. Either a single value or one for every dimension
censor_range	Uncertainty range for censoring. A length-2-vector of certainty range start and end. TODO: also allow $2 \times G$ matrix
missing_range	Whole data range for missing value model. Has to be specified if NAs are in the data
vars	Variables (columns) of the data to use. Specifying TRUE will select all columns (default: All floating point value columns)
verbose	logical. If TRUE, show a progress bar and plot the output

Value

Object of class [Sigmas](#)

See Also

[Sigmas](#), the class returned by this; [DiffusionMap](#), the class this is used for

Examples

```
data(guo)
sigs <- find_sigmas(guo, verbose = TRUE)
DiffusionMap(guo, sigs)
```

find_tips

Find tips in a DiffusionMap object

Description

Find tips in a DiffusionMap object

Usage

```
find_tips(dm_or_dpt, root = random_root(dm_or_dpt))
```

Arguments

dm_or_dpt A [DiffusionMap](#) or [DPT](#) object
 root Root cell index from which to find tips. (default: random)

Value

An integer vector of length 3

Examples

```
data(guo)
dm <- DiffusionMap(guo)
is_tip <- l_which(find_tips(dm), len = ncol(guo))
plot(dm, col = factor(is_tip))
```

Gene Relevance

Gene relevances for entire data set

Description

The relevance map is cached insided of the [DiffusionMap](#).

Usage

```
gene_relevance(coords, exprs, ..., k = 20L, dims = 1:2, distance = NULL,
  smooth = TRUE, verbose = FALSE)
```

```
## S4 method for signature 'DiffusionMap,missing'
gene_relevance(coords, exprs, ..., k = 20L,
  dims = 1:2, distance = NULL, smooth = TRUE, verbose = FALSE)
```

```
## S4 method for signature 'matrix,matrix'
gene_relevance(coords, exprs, ..., k = 20L,
  dims = 1:2, distance = NULL, smooth = TRUE, verbose = FALSE)
```

Arguments

coords A [DiffusionMap](#) object or a cells \times dims [matrix](#).
 exprs An cells \times genes [matrix](#). Only provide if coords is no [DiffusionMap](#).
 ... If no [DiffusionMap](#) is provided, a vector of weights (of the same length as
 dims) can be provided.
 k Number of nearest neighbors to use
 dims Index into columns of coord
 distance Distance measure to use for the nearest neighbor search.
 smooth Smoothing parameters c(window, alpha) (see [smth.gaussian](#)). Alternatively
 [TRUE](#) to use the [smoother defaults](#) or [FALSE](#) to skip smoothing,
 verbose If [TRUE](#), log additional info to the console

Value

A GeneRelevance object:

Slots

`coords` A $\text{cells} \times \text{dims}$ `matrix` or `sparseMatrix` of coordinates (e.g. diffusion components), reduced to the dimensions passed as `dims`

`exprs` A $\text{cells} \times \text{genes}$ matrix of expressions

`partials` Array of partial derivatives wrt to considered dimensions in reduced space ($\text{genes} \times \text{cells} \times \text{dimensions}$)

`partials_norm` Matrix with norm of aforementioned derivatives. ($n \setminus \text{genes} \times \text{cells}$)

`nn_index` Matrix of `k` nearest neighbor indices. ($\text{cells} \times k$)

`dims` Column index for plotted dimensions. Can be `character`, `numeric` or `logical`

`distance` Distance measure used in the nearest neighbor search. See `find_knn`

`smooth_window` Smoothing window used (see `smth.gaussian`)

`smooth_alpha` Smoothing kernel width used (see `smth.gaussian`)

See Also

[Gene Relevance methods](#), [Gene Relevance plotting](#): `plot_differential_map/plot_gene_relevance`

Examples

```
data(guo_norm)
dm <- DiffusionMap(guo_norm)
gr <- gene_relevance(dm)

m <- t(Biobase::exprs(guo_norm))
gr_pca <- gene_relevance(prcomp(m)$x, m)
# now plot them!
```

Gene Relevance methods

Gene Relevance methods

Description

`featureNames <- ...` Can be used to set the gene names used for plotting (e.g. if the data contains hardly readable gene or transcript IDs)

Usage

```
## S4 method for signature 'GeneRelevance'
featureNames(object)

## S4 replacement method for signature 'GeneRelevance,characterOrFactor'
featureNames(object) <- value
```

```
## S4 method for signature 'GeneRelevance'
dataset(object)

## S4 replacement method for signature 'GeneRelevance'
dataset(object) <- value
```

Arguments

object [GeneRelevance](#) object
value A text vector ([character](#) or [factor](#))

See Also

[gene_relevance](#), [Gene Relevance plotting](#)

Examples

```
data(guo_norm)
gr <- gene_relevance(DiffusionMap(guo_norm))
featureNames(gr)[[37]] <- 'Id2 (suppresses differentiation)'
# now plot it with the changed gene name(s)
```

Gene Relevance plotting

Plot gene relevance or differential map

Description

`plot(gene_relevance, 'Gene')` plots the differential map of this/these gene(s), `plot(gene_relevance)` a relevance map of a selection of genes. Alternatively, you can use `plot_differential_map` or `plot_gene_relevance` on a [GeneRelevance](#) or [DiffusionMap](#) object, or with two matrices.

Usage

```
## S4 method for signature 'GeneRelevance,character'
plot(x, y, ...)

## S4 method for signature 'GeneRelevance,numeric'
plot(x, y, ...)

## S4 method for signature 'GeneRelevance,missing'
plot(x, y, ...)

plot_differential_map(coords, exprs, ..., gene, dims = 1:2,
  pal = cube_helix, faceter = facet_wrap(~Gene))

## S4 method for signature 'matrix,matrix'
plot_differential_map(coords, exprs, ..., gene,
  dims = 1:2, pal = cube_helix, faceter = facet_wrap(~Gene))

## S4 method for signature 'DiffusionMap,missing'
```

```

plot_differential_map(coords, exprs, ..., gene,
  dims = 1:2, pal = cube_helix, faceter = facet_wrap(~Gene))

## S4 method for signature 'GeneRelevance,missing'
plot_differential_map(coords, exprs, ...,
  gene, dims = 1:2, pal = cube_helix, faceter = facet_wrap(~Gene))

plot_gene_relevance(coords, exprs, ..., iter_smooth = 2L, genes = 5L,
  dims = 1:2, pal = palette())

## S4 method for signature 'matrix,matrix'
plot_gene_relevance(coords, exprs, ...,
  iter_smooth = 2L, genes = 5L, dims = 1:2, pal = palette())

## S4 method for signature 'DiffusionMap,missing'
plot_gene_relevance(coords, exprs, ...,
  iter_smooth = 2L, genes = 5L, dims = 1:2, pal = palette())

## S4 method for signature 'GeneRelevance,missing'
plot_gene_relevance(coords, exprs, ...,
  iter_smooth = 2L, genes = 5L, dims = 1:2, pal = palette())

```

Arguments

x	GeneRelevance object.
y, gene	Gene name(s) or index/indices to create differential map for. (integer or character)
...	Passed to <code>plot_differential_map/plot_gene_relevance</code> .
coords	A DiffusionMap/GeneRelevance object or a cells \times dims matrix .
exprs	An cells \times genes matrix . Only provide if coords is a matrix.
dims	Names or indices of dimensions to plot. When not plotting a GeneRelevance object, the relevance for the dimensions 1:max(dims) will be calculated.
pal	Palette. Either A colormap function or a list of colors.
faceter	A ggplot faceter like <code>facet_wrap(~ Gene)</code> .
iter_smooth	Number of label smoothing iterations to perform on relevance map. The higher the more homogenous and the less local structure.
genes	Genes to based relevance map on or number of genes to use. (vector of strings or one number) You can also pass an index into the gene names. (vector of numbers or logicals with length > 1)

Value

ggplot2 plot, when plotting a relevance map with a list member `$ids` containing the gene IDs used.

See Also

[gene_relevance](#), [Gene Relevance methods](#)

Examples

```
data(guo_norm)
dm <- DiffusionMap(guo_norm)
gr <- gene_relevance(dm)
plot(gr) # or plot_gene_relevance(dm)
plot(gr, 'Fgf4') # or plot_differential_map(dm, 'Fgf4')

guo_norm_mat <- t(Biobase::exprs(guo_norm))
pca <- prcomp(guo_norm_mat)$x
plot_gene_relevance(pca, guo_norm_mat, dims = 2:3)
plot_differential_map(pca, guo_norm_mat, gene = c('Fgf4', 'Nanog'))
```

guo

Guo et al. mouse embryonic stem cell qPCR data

Description

Gene expression data of 48 genes and an annotation column `$num_cells` containing the cell stage at which the embryos were harvested.

Usage

```
data(guo)
data(guo_norm)
```

Format

An [ExpressionSet](#) with 48 features, 428 observations and 2 [phenoData](#) annotations.

Details

The data is normalized using the mean of two housekeeping genes. The difference between `guo` and `guo_norm` is the LoD being set to 10 in the former, making it usable with the `sensor_val` parameter of [DiffusionMap](#).

Value

an [ExpressionSet](#) with 48 features and 428 observations containing qPCR Ct values and a "num.cells" observation annotation.

Author(s)

Guoji Guo, Mikael Huss, Guo Qing Tong, Chaoyang Wang, Li Li Sun, Neil D. Clarke, Paul Robson
<robsonp@gis.a-star.edu.sg>

References

<http://www.sciencedirect.com/science/article/pii/S1534580710001103>

knn	<i>kNN search</i>
-----	-------------------

Description

k nearest neighbor search with custom distance function.

Usage

```
find_knn(data, k, ..., query = NULL, distance = c("euclidean", "cosine",
"rankcor"), sym = TRUE)
```

Arguments

data	Data matrix
k	Number of nearest neighbors
...	Unused. All parameters to the right of the ... have to be specified by name (e.g. <code>find_knn(data,k,distance = 'cosine')</code>)
query	Query matrix. In <code>knn</code> and <code>knn_asym</code> , query and data are identical
distance	Distance metric to use. Allowed measures: Euclidean distance (default), cosine distance ($1 - \text{corr}(c_1, c_2)$) or rank correlation distance ($1 - \text{corr}(\text{rank}(c_1), \text{rank}(c_2))$)
sym	Return a symmetric matrix (as long as query is NULL)?

Value

A `dgCMatrix` if `sym == TRUE`, else a `dsCMatrix` ($nrow(query) \times nrow(data)$).

l_which	<i>Logical which</i>
---------	----------------------

Description

Inverse of `which`. Converts an array of numeric or character indices to a logical index array. This function is useful if you need to perform logical operation on an index array but are only given numeric indices.

Usage

```
l_which(idx, nms = seq_len(len), len = length(nms), useNames = TRUE)
```

Arguments

idx	Numeric or character indices.
nms	Array of names or a sequence. Required if <code>idx</code> is a character array
len	Length of output array. Alternative to <code>nms</code> if <code>idx</code> is numeric
useNames	Use the names of <code>nms</code> or <code>idx</code>

Details

Either nms or len has to be specified.

Value

Logical vector of length len or the same length as nms

Examples

```
all(1_which(2, len = 3L) == c(FALSE, TRUE, FALSE))
all(1_which(c('a', 'c'), letters[1:3]) == c(TRUE, FALSE, TRUE))
```

plot.DiffusionMap	<i>3D or 2D plot of diffusion map</i>
-------------------	---------------------------------------

Description

If you want to plot the eigenvalues, simply `plot(eigenvalues(dm)[start:end], ...)`

Usage

```
plot.DiffusionMap(x, dims = 1:3, new_dcs = if (!is.null(new_data))
  dm_predict(x, new_data), new_data = NULL, col = NULL, col_by = NULL,
  col_limits = NULL, col_new = "red", pal = NULL, pal_new = NULL, ...,
  ticks = FALSE, axes = TRUE, box = FALSE, legend_main = col_by,
  legend_opts = list(), interactive = FALSE,
  draw_legend = !is.null(col_by) || (length(col) > 1 && !is.character(col)),
  consec_col = TRUE, col_na = "grey", plot_more = function(p, ..., rescale
  = NULL) p)
```

```
## S4 method for signature 'DiffusionMap,numeric'
plot(x, y, ...)
```

```
## S4 method for signature 'DiffusionMap,missing'
plot(x, y, ...)
```

Arguments

x	A DiffusionMap
dims, y	Diffusion components (eigenvectors) to plot (default: first three components; 1:3)
new_dcs	An optional matrix also containing the rows specified with y and plotted. (default: no more points)
new_data	A data set in the same format as x that is used to create <code>new_dcs <- dm_predict(dif, new_data)</code>
col	Single color string or vector of discrete or categoric values to be mapped to colors. E.g. a column of the data matrix used for creation of the diffusion map. (default: cluster_louvain)
col_by	Specify a <code>dataset(x)</code> or <code>phenoData(dataset(x))</code> column to use as color

col_limits	If col is a continuous (=double) vector, this can be overridden to map the color range differently than from min to max (e.g. specify <code>c(0, 1)</code>)
col_new	If new_dcs is given, it will take on this color. A vector is also possible. (default: red)
pal	Palette used to map the col vector to colors. (default: use <code>cube_helix</code> for continuous and <code>palette()</code> for discrete data)
pal_new	Palette used to map the col_new vector to colors. (default: see pal argument)
...	Parameters passed to <code>plot</code> , <code>scatterplot3d</code> , or <code>plot3d</code> (if <code>interactive == TRUE</code>)
ticks	logical. If TRUE, show axis ticks (default: FALSE)
axes	logical. If TRUE, draw plot axes (default: Only if ticks is TRUE)
box	logical. If TRUE, draw plot frame (default: TRUE or the same as axes if specified)
legend_main	Title of legend. (default: nothing unless col_by is given)
legend_opts	Other <code>colorlegend</code> options (default: empty list)
interactive	Use <code>plot3d</code> to plot instead of <code>scatterplot3d</code> ?
draw_legend	logical. If TRUE, draw color legend (default: TRUE if col_by is given or col is given and a vector to be mapped)
consec_col	If col or col_by refers to an integer column, with gaps (e.g. <code>c(5, 0, 0, 3)</code>) use the palette color consecutively (e.g. <code>c(3, 1, 1, 2)</code>)
col_na	Color for NA in the data. specify NA to hide.
plot_more	Function that will be called while the plot margins are temporarily changed (its p argument is the rgl or scatterplot3d instance or NULL, its rescale argument is NULL, a <code>list(from = c(a, b), to = c(c, d))</code>), or an array of shape <code>from to × dims × min max</code> , i.e. $2 \times length(dims) \times 2$. In case of 2d plotting, it should take and return a <code>ggplot2</code> object.

Details

If you specify negative numbers as diffusion components (e.g. `plot(dm, c(-1, 2))`), then the corresponding components will be flipped.

Value

The return value of the underlying call is returned, i.e. a `scatterplot3d` or `rgl` object.

Examples

```
data(guo)
plot(DiffusionMap(guo))
```

plot.DPT

*Plot DPT***Description**

Plots diffusion components from a Diffusion Map and the accompanying Diffusion Pseudo Time (DPT)

Usage

```
plot.DPT(x, root = NULL, paths_to = integer(0L), dcs = 1:2,
         divide = integer(0L), w_width = 0.1, col_by = "dpt",
         col_path = rev(palette()), col_tip = "red", ..., col = NULL,
         legend_main = col_by)
```

```
## S4 method for signature 'DPT,numeric'
plot(x, y, ...)
```

```
## S4 method for signature 'DPT,missing'
plot(x, y, ...)
```

Arguments

x	A DPT object.
paths_to	Numeric Branch IDs. Are used as target(s) for the path(s) to draw.
dcs	The dimensions to use from the DiffusionMap
divide	If col_by = 'branch', this specifies which branches to divide. (see branch_divide)
w_width	Window width for smoothing the path (see smth.gaussian)
col_by	Color by 'dpt' (DPT starting at branches[[1]]), 'branch', or a variable of the data.
col_path	Colors for the path or a function creating n colors
col_tip	Color for branch tips
...	Graphical parameters supplied to plot.DiffusionMap
col	See plot.DiffusionMap . This overrides col_by
legend_main	See plot.DiffusionMap .
y, root	Root branch ID. Will be used as the start of the DPT. (default: lowest branch ID) (If longer than size 1, will be interpreted as c(root, branches))

Value

The return value of the underlying call is returned, i.e. a scatterplot3d or rgl object for 3D plots.

Examples

```

data(guo_norm)
dm <- DiffusionMap(guo_norm)
dpt <- DPT(dm)
plot(dpt)
plot(dpt, 2L, col_by = 'branch')
plot(dpt, 1L, 2:3, col_by = 'num_cells')
plot(dpt, col_by = 'DPT3')

```

plot.Sigmas	<i>Plot Sigmas object</i>
-------------	---------------------------

Description

Plot [Sigmas](#) object

Usage

```

## S4 method for signature 'Sigmas,missing'
plot(x, col = par("fg"),
     col_highlight = "#E41A1C", col_line = "#999999", type = c("b", "b"),
     pch = c(par("pch"), 4L), only_dim = FALSE, ..., xlab = NULL,
     ylab = NULL, main = "")

```

Arguments

x	Sigmas object to plot
col	Vector of bar colors or single color for all bars
col_highlight	Color for highest bar. Overrides col
col_line	Color for the line and its axis
type	Plot type of both lines. Can be a vector of length 2 to specify both separately (default: 'b' aka "both lines and points")
pch	Point identifier for both lines. Can be a vector of length 2 to specify both separately (default: par(pch) and 4 (a 'x'))
only_dim	logical. If TRUE, only plot the derivative line
...	Options passed to the call to plot
xlab	X label. NULL to use default
ylab	Either one y label or y labels for both plots. NULL to use both defaults, a NULL in a list of length 2 to use one default.
main	Title of the plot

Value

This method plots a Sigma object to the current device and returns nothing/NULL

Examples

```
data(guo)
sigs <- find_sigmas(guo)
plot(sigs)
```

projection_dist	<i>Projection distance</i>
-----------------	----------------------------

Description

Projection distance

Usage

```
projection_dist(dm, new_dcs = NULL, ..., new_data, verbose = FALSE)
```

Arguments

dm	A DiffusionMap object.
new_dcs	Diffusion component matrix of which to calculate the distance to the data.
...	Passed to proxy::dist if new_data was passed.
new_data	New data points to project into the diffusion map. Can be a matrix , data.frame , ExpressionSet , or SingleCellExperiment .
verbose	If TRUE , log additional info to the console.

Examples

```
data(guo_norm)
g2_32 <- guo_norm[, guo_norm$num_cells < 64]
g64 <- guo_norm[, guo_norm$num_cells == 64]
dm <- DiffusionMap(g2_32)
d <- projection_dist(dm, new_data = g64)
```

random_root	<i>Find a random root cell index</i>
-------------	--------------------------------------

Description

Finds a cell that has the maximum DPT distance from a randomly selected one.

Usage

```
random_root(dm_or_dpt)
```

Arguments

dm_or_dpt	A DiffusionMap or DPT object
-----------	--

Value

A cell index

Examples

```
data(guo)
dm <- DiffusionMap(guo)
random_root(dm)
```

Sigmas class

Sigmas Object

Description

Holds the information about how the `sigma` parameter for a [DiffusionMap](#) was obtained, and in this way provides a plotting function for the [find_sigmas](#) heuristic. You should not need to create a `Sigmas` object yourself. Provide `sigma` to [DiffusionMap](#) instead or use [find_sigmas](#).

Usage

```
Sigmas(...)

## S4 method for signature 'Sigmas'
optimal_sigma(object)

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

## S4 method for signature 'Sigmas'
show(object)
```

Arguments

`object, x` [Sigmas](#) object
`...` See “**Slots**” below

Details

A `Sigmas` object is either created by [find_sigmas](#) or by specifying the `sigma` parameter to [DiffusionMap](#).

In the second case, if the `sigma` parameter is just a number, the resulting `Sigmas` object has all slots except of `optimal_sigma` set to `NULL`.

Value

`Sigmas` creates an object of the same class

`optimal_sigma` retrieves the numeric value of the optimal sigma or local sigmas

Slots

log_sigmas Vector of length m containing the \log_{10} of the σ s
dim_norms Vector of length $m - 1$ containing the average dimensionality $\langle p \rangle$ for the respective kernel widths
optimal_sigma Multiple local sigmas or the mean of the two global σ s around the highest $\langle p \rangle$ (`c(optimal_idx, optimal_idx+1L)`)
optimal_idx The index of the highest $\langle p \rangle$.
avrd_norms Vector of length m containing the average dimensionality for the corresponding sigma.

See Also

[find_sigmas](#), the function to determine a locally optimal sigma and returning this class

Examples

```

data(guo)
sigs <- find_sigmas(guo, verbose = FALSE)
optimal_sigma(sigs)
print(sigs)

```

updateObject-method *Update old destiny objects to a newer version.*

Description

Handles [DiffusionMap](#), [Sigmas](#), and [GeneRelevance](#).

Usage

```

## S4 method for signature 'DiffusionMap'
updateObject(object, ..., verbose = FALSE)

## S4 method for signature 'Sigmas'
updateObject(object, ..., verbose = FALSE)

## S4 method for signature 'GeneRelevance'
updateObject(object, ..., verbose = FALSE)

```

Arguments

<code>object</code>	An object created with an older destiny release
<code>...</code>	ignored
<code>verbose</code>	tells what is being updated

Value

A [DiffusionMap](#) or [Sigmas](#) object that is valid when used with the current destiny release

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