Package 'densityratio'

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Type Package

Title Distribution Comparison Through Density Ratio Estimation

Version 0.2.0

Description Fast, flexible and user-friendly tools for distribution comparison through direct density ratio estimation. The estimated density ratio can be used for covariate shift adjustment, outlier-detection, change-point detection, classification and evaluation of synthetic data quality. The package implements multiple non-parametric estimation techniques (unconstrained least-squares importance fitting, ulsif(), Kullback-Leibler importance estimation procedure, kliep(), spectral density ratio estimation, spectral(), kernel mean matching, kmm(), and least-squares hetero-distributional subspace search, lhss()). with automatic tuning of hyperparameters. Helper functions are available for two-sample testing and visualizing the density ratios. For an overview on density ratio estimation, see Sugiyama et al. (2012) <doi:10.1017/CBO9781139035613> for a general overview, and the help files for references on the specific estimation techniques.

License GPL (>= 3) Encoding UTF-8

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Description

Colon cancer data set from princeton, containing 2000 gene expressions from 22 colon tumor tissues and 40 non-tumor tissues. The data is collected by Alon et al. (1999) and can be obtained from here.

Format

A data.frame with 62 rows and 2001 columns (class variable and 2000 gene expressions).

```
create_bivariate_plot Bivariate plot
```

Description

Bivariate plot

Usage

```
create_bivariate_plot(data, ext, vars, logscale, show.sample)
```

Arguments

data	Data frame with the individual values and density ratio estimates
ext	Data frame with the density ratio estimates and sample indicator
vars	Character vector of variable names to be plotted.
logscale	Logical indicating whether the density ratio should be plotted in log scale. Defaults to TRUE.
show.sample	Logical indicating whether to give different shapes to observations, depending on the sample they come from (numerator or denominator). Defaults to FALSE.

Value

Bivariate plot

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create_univariate_plot

Univariate plot

Description

Scatterplot of individual values and density ratio estimates. Used internally in create_univariate_plot()

Usage

```
create_univariate_plot(data, ext, var, y_lab, sample.facet = TRUE)
```

Arguments

data	Data frame with the individual values and density ratio estimates
ext	Data frame with the density ratio estimates and sample indicator
var	Name of the variable to be plotted on the x-axis

y_lab Name of the y-axis label, typically ("Density Ratio" or "Log Density Ratio") sample. facet Logical indicating whether to facet the plot by sample. Default is TRUE.

Value

A scatterplot of variable values and density ratio estimates.

Description

Simulated data set (see data-raw/generate-data-densityratio.R) with five variables that are used in the examples.

Format

A data frame with 1000 rows and 5 columns:

- x1 Categorical variable with three categories, 'A', 'B' and 'C'
- x2 Categorical variable with two categories, 'G1' and 'G2'
- x3 Continuous variable (normally distributed given x1 and x2)
- x4 Continuous variable (normally distributed)
- x5 Continuous variable (normally distributed)

denominator_small 5

_small <i>denominator_small</i>

Description

Subset of the denominator_data with three variables and 50 observations

Format

A data frame with 100 rows and 3 columns:

- x1 Continuous variable (normally distributed given x1 and x2)
- x2 Continuous variable (normally distributed)
- x3 Continuous variable (normally distributed)

distance	Create a Gram matrix with squared Euclidean distances between ob-
	servations in the input matrix X and the input matrix Y

Description

Create a Gram matrix with squared Euclidean distances between observations in the input matrix X and the input matrix Y

Arguments

V A numaria input m	
X A numeric input m	ашіл

Y A numeric input matrix with the same variables as X

intercept Logical indicating whether an intercept should be added to the estimation pro-

cedure. In this case, the first column is an all-zero column (which will be trans-

formed into an all-ones column in the kernel).

dr.histogram

dr.histogram

A histogram of density ratio estimates

Description

Creates a histogram of the density ratio estimates. Useful to understand the distribution of estimated density ratios in each sample, or compare it among samples. It is the default plotting method for density ratio objects.

Usage

```
dr.histogram(
  samples = "both",
  logscale = TRUE,
  binwidth = NULL,
 bins = NULL,
  tol = 0.01,
)
## S3 method for class 'ulsif'
plot(
  Х,
  samples = "both",
  logscale = TRUE,
  binwidth = NULL,
 bins = NULL,
  tol = 0.01,
)
## S3 method for class 'kliep'
plot(
 х,
  samples = "both",
  logscale = TRUE,
  binwidth = NULL,
  bins = NULL,
  tol = 0.01,
)
## S3 method for class 'kmm'
plot(
  Х,
  samples = "both",
```

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```
logscale = TRUE,
 binwidth = NULL,
 bins = NULL,
  tol = 0.01,
)
## S3 method for class 'spectral'
plot(
 samples = "both",
 logscale = TRUE,
 binwidth = NULL,
 bins = NULL,
  tol = 0.01,
)
## S3 method for class 'lhss'
plot(
 х,
  samples = "both",
 logscale = TRUE,
 binwidth = NULL,
 bins = NULL,
  tol = 0.01,
)
## S3 method for class 'naivedensityratio'
plot(
 х,
  samples = "both",
 logscale = TRUE,
 binwidth = NULL,
 bins = NULL,
  tol = 0.01,
)
```

Arguments

Χ	Density ratio object created with e.g., kliep(), ulsif(), or naive()
samples	Character string indicating whether to plot the 'numerator', 'denominator', or 'both' samples. Default is 'both'.
logscale	Logical indicating whether to plot the density ratio estimates on a log scale. Default is TRUE.
binwidth	Numeric indicating the width of the bins, passed on to ggplot2.

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bins	Numeric indicating the number of bins. Overriden by binwidth, and passed on to ggplot2.
tol	Numeric indicating the tolerance: values below this value will be set to the tolerance value, for legibility of the plots
	Additional arguments passed on to predict().

Value

A histogram of density ratio estimates.

See Also

```
ulsif for example usage
kliep for example usage
kmm for example usage
spectral for example usage
lhss for example usage
naive for example usage
```

insurance

insurance

Description

Insurance data that is openly available (e.g., on Kaggle).

Format

A data.frame with 1338 rows and 7 columns:

age Age of the insured (continuous)

sex Sex of the insured (binary)

bmi Body mass index of the insured (continuous)

children Number of children/dependents covered by the insurance (integer)

smoker Whether the insured is a smoker (binary)

region The region in which the insured lives (categorical)

charges The medical costs billed by the insurance (continuous)

kernel_gaussian 9

kernel_gaussian	Create gaussian kernel gram matrix from distance matrix

Description

Create gaussian kernel gram matrix from distance matrix

Arguments

Arguments	
dist	A numeric distance matrix
sigma	A scalar with the length-scale parameter
kidiq	kidiq

Description

The kidiq data stems from the National Longitudinal Survey of Youth and is used in Gelman and Hill (2007). The data set contains 434 observations measured on five variables, and is obtained from https://github.com/jknowles/BDAexampleR.

Format

A data.frame with 434 rows and 5 columns

mom_iq Mother's IQ score (continuous)

```
kid_score Child's IQ score (continuous)mom_hs Whether the mother obtained a high school degree (binary)
```

mom_work Whether the mother worked in the first three years of the child's life (1: not in the first three years; 2: in the second or third year; 3: parttime in the first year; 4: fulltime in the first year)

mom_age Mother's age (continuous)

10 kliep

kliep

Kullback-Leibler importance estimation procedure

Description

Kullback-Leibler importance estimation procedure

Usage

```
kliep(
  df_numerator,
  df_denominator,
  scale = "numerator",
  nsigma = 10,
  sigma_quantile = NULL,
  sigma = NULL,
  ncenters = 200,
  centers = NULL,
  cv = TRUE,
  nfold = 5,
  epsilon = NULL,
  maxit = 5000,
  progressbar = TRUE
)
```

Arguments

df_numerator	data.frame with exclusively numeric variables with the numerator samples
df_denominator	data.frame with exclusively numeric variables with the denominator samples (must have the same variables as df_denominator)
scale	"numerator", "denominator", or NULL, indicating whether to standardize each numeric variable according to the numerator means and standard deviations, the denominator means and standard deviations, or apply no standardization at all.
nsigma	Integer indicating the number of sigma values (bandwidth parameter of the Gaussian kernel gram matrix) to use in cross-validation.
sigma_quantile	NULL or numeric vector with probabilities to calculate the quantiles of the distance matrix to obtain sigma values. If NULL, nsigma values between 0.25 and 0.75 are used.
sigma	NULL or a scalar value to determine the bandwidth of the Gaussian kernel gram matrix. If NULL, nsigma values between 0.25 and 0.75 are used.
ncenters	Maximum number of Gaussian centers in the kernel gram matrix. Defaults to all numerator samples.
centers	Option to specify the Gaussian samples manually.
cv	Logical indicating whether or not to do cross-validation

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nfold	Number of cross-validation folds used in order to calculate the optimal sigma value (default is 5-fold cv).
epsilon	Numeric scalar or vector with the learning rate for the gradient-ascent procedure. If a vector, all values are used as the learning rate. By default, $10^{1:-5}$ is used.
maxit	Maximum number of iterations for the optimization scheme.
progressbar	Logical indicating whether or not to display a progressbar.

Value

kliep-object, containing all information to calculate the density ratio using optimal sigma and optimal weights.

References

Sugiyama, M., Suzuki, T., Nakajima, S., Kashima, H., Von Bünau, P., & Kawanabe, M. (2008). Direct importance estimation for covariate shift adaptation. Annals of the Institute of Statistical Mathematics 60, 699-746. Doi: https://doi.org/10.1007/s10463-008-0197-x.

Examples

```
set.seed(123)
# Fit model
dr <- kliep(numerator_small, denominator_small)</pre>
# Inspect model object
dr
# Obtain summary of model object
summary(dr)
# Plot model object
plot(dr)
# Plot density ratio for each variable individually
plot_univariate(dr)
# Plot density ratio for each pair of variables
plot_bivariate(dr)
# Predict density ratio and inspect first 6 predictions
head(predict(dr))
# Fit model with custom parameters
kliep(numerator_small, denominator_small,
      nsigma = 1, ncenters = 100, nfold = 10,
      epsilon = 10^{2:-5}, maxit = 500)
```

kmm

Kernel mean matching approach to density ratio estimation

Description

Kernel mean matching approach to density ratio estimation

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Usage

```
kmm(
  df_numerator,
  df_denominator,
  scale = "numerator",
  constrained = FALSE,
  nsigma = 10,
  sigma_quantile = NULL,
  sigma = NULL,
  ncenters = 200,
  centers = NULL,
  cv = TRUE,
  nfold = 5,
  parallel = FALSE,
  nthreads = NULL,
  progressbar = TRUE,
 osqp_settings = NULL,
  cluster = NULL
)
```

Arguments

df_numerator	data.frame with exclusively numeric variables with the numerator samples
df_denominator	data.frame with exclusively numeric variables with the denominator samples (must have the same variables as df_denominator)
scale	"numerator", "denominator", or NULL, indicating whether to standardize each numeric variable according to the numerator means and standard deviations, the denominator means and standard deviations, or apply no standardization at all.
constrained	logical equals FALSE to use unconstrained optimization, TRUE to use constrained optimization. Defaults to FALSE.
nsigma	Integer indicating the number of sigma values (bandwidth parameter of the Gaussian kernel gram matrix) to use in cross-validation.
sigma_quantile	NULL or numeric vector with probabilities to calculate the quantiles of the distance matrix to obtain sigma values. If NULL, nsigma values between 0.25 and 0.75 are used.
sigma	NULL or a scalar value to determine the bandwidth of the Gaussian kernel gram matrix. If NULL, nsigma values between 0.25 and 0.75 are used.
ncenters	Maximum number of Gaussian centers in the kernel gram matrix. Defaults to all numerator samples.
centers	Option to specify the Gaussian samples manually.
CV	Logical indicating whether or not to do cross-validation
nfold	Number of cross-validation folds used in order to calculate the optimal sigma value (default is 5-fold cv).
parallel	logical indicating whether to use parallel processing in the cross-validation scheme.

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nthreads NULL or integer indicating the number of threads to use for parallel processing.

If parallel processing is enabled, it defaults to the number of available threads

minus one.

progressbar Logical indicating whether or not to display a progressbar.

osqp_settings Optional: settings to pass to the osqp solver for constrained optimization.

cluster Optional: a cluster object to use for parallel processing, see parallel::makeCluster.

Value

kmm-object, containing all information to calculate the density ratio using optimal sigma and optimal weights.

References

Huang, J., Smola, A. J., Gretton, A., Borgwardt, K. M., & Schölkopf, B. (2006). Correcting sample selection bias by unlabeled data. In Advances in Neural Information Processing Systems, edited by B. Schölkopf, J. Platt and T. Hoffman. Available from https://proceedings.neurips.cc/paper/2006/hash/a2186aa7c086b46ad4e8bf81e2a3a19b-Abstract.html.

Examples

```
set.seed(123)
# Fit model
dr <- kmm(numerator_small, denominator_small)</pre>
# Inspect model object
dr
# Obtain summary of model object
summary(dr)
# Plot model object
plot(dr)
# Plot density ratio for each variable individually
plot_univariate(dr)
# Plot density ratio for each pair of variables
plot_bivariate(dr)
# Predict density ratio and inspect first 6 predictions
head(predict(dr))
# Fit model with custom parameters
kmm(numerator_small, denominator_small,
    nsigma = 5, ncenters = 100, nfold = 10,
    constrained = TRUE)
```

lhss

Least-squares heterodistributional subspace search

Description

Least-squares heterodistributional subspace search

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Usage

```
lhss(
  df_numerator,
 df_denominator,
 m = NULL,
 intercept = TRUE,
  scale = "numerator",
  nsigma = 10,
  sigma_quantile = NULL,
  sigma = NULL,
  nlambda = 10,
  lambda = NULL,
 ncenters = 200,
 centers = NULL,
 maxit = 200,
 progressbar = TRUE
)
```

Arguments

progressbar

df_numerator	data.frame with exclusively numeric variables with the numerator samples
df_denominator	$\label{lem:data:frame} \begin{picture}(100,0) \put(0,0){\line(0,0){100}} \put(0,0){\line(0,0){100}$
m	Scalar indicating the dimensionality of the reduced subspace
intercept	logical Indicating whether to include an intercept term in the model. Defaults to TRUE.
scale	"numerator", "denominator", or NULL, indicating whether to standardize each numeric variable according to the numerator means and standard deviations, the denominator means and standard deviations, or apply no standardization at all.
nsigma	Integer indicating the number of sigma values (bandwidth parameter of the Gaussian kernel gram matrix) to use in cross-validation.
sigma_quantile	NULL or numeric vector with probabilities to calculate the quantiles of the distance matrix to obtain sigma values. If NULL, nsigma values between 0.05 and 0.95 are used.
sigma	NULL or a scalar value to determine the bandwidth of the Gaussian kernel gram matrix. If NULL, nsigma values between 0.05 and 0.95 are used.
nlambda	Integer indicating the number of lambda values (regularization parameter), by default, lambda is set to $10^seq(3, -3, length.out = nlambda)$.
lambda	NULL or numeric vector indicating the lambda values to use in cross-validation
ncenters	Maximum number of Gaussian centers in the kernel gram matrix. Defaults to all numerator samples.
centers	Numeric matrix with the same variables as nu and de that are used as Gaussian centers in the kernel Gram matrix. By default, the matrix nu is used as the matrix with Gaussian centers.
maxit	Maximum number of iterations in the updating scheme.

Logical indicating whether or not to display a progressbar.

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Value

lhss-object, containing all information to calculate the density ratio using optimal sigma, optimal lambda and optimal weights.

References

Sugiyama, M., Yamada, M., Von Bünau, P., Suzuki, T., Kanamori, T. & Kawanabe, M. (2011). Direct density-ratio estimation with dimensionality reduction via least-squares hetero-distributional subspace search. Neural Networks, 24, 183-198. doi:10.1016/j.neunet.2010.10.005.

Examples

```
set.seed(123)
# Fit model
dr <- naive(numerator_small, denominator_small)</pre>
# Inspect model object
# Obtain summary of model object
summary(dr)
# Plot model object
plot(dr)
# Plot density ratio for each variable individually
plot_univariate(dr)
# Plot density ratio for each pair of variables
plot_bivariate(dr)
# Predict density ratio and inspect first 6 predictions
head(predict(dr))
# Fit model with custom parameters
naive(numerator_small, denominator_small, m=2, kernel="epanechnikov")
```

naive

Naive density ratio estimation

Description

The naive approach creates separate kernel density estimates for the numerator and the denominator samples, and then evaluates their ratio for the denominator samples. For multivariate data, the density ratio is computed after a orthogonal linear transformation, such that the new variables can be treated as independent. To reduce the dimensionality of the PCA solution, one can set the number of components by setting the m parameter to an integer value smaller than the number of variables.

Usage

```
naive(
  df_numerator,
  df_denominator,
  m = NULL,
  bw = "SJ",
```

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```
kernel = "gaussian",
    n = 2L^11,
    ...
)
```

Arguments

m

df_numerator data.frame with exclusively numeric variables with the numerator samples df_denominator data.frame with exclusively numeric variables with the denominator samples

(must have the same variables as df_denominator)

integer Optional parameter to reduce the dimensionality of the data in multivariate density ratio estimation problems. If missing, the number of variables in the data is used. If set to an integer value smaller than the number of variables, the first m principal components are used to estimate the density ratio. If set to NULL, the square root of the number of variables is used (for consistency with

other methods).

bw the smoothing bandwidth to be used. See stats::density for more information.

kernel the kernel to be used. See stats::density for more information.

integer the number of equally spaced points at which the density is to be es-

timated. When n > 512, it is rounded up to a power of 2 during the calculations (as fast Fourier transform is used) and the final result is interpolated by

stats::approx. So it makes sense to specify n as a power' of two.

... further arguments passed to stats::density

Value

naivedensityratio object

See Also

```
stats::density()
```

```
set.seed(123)
# Fit model
dr <- naive(numerator_small, denominator_small)
# Inspect model object
dr
# Obtain summary of model object
summary(dr)
# Plot model object
plot(dr)
# Plot density ratio for each variable individually
plot_univariate(dr)
# Plot density ratio for each pair of variables
plot_bivariate(dr)
# Predict density ratio and inspect first 6 predictions
head(predict(dr))</pre>
```

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```
# Fit model with custom parameters
naive(numerator_small, denominator_small, m=2, kernel="epanechnikov")
```

numerator_data

numerator_data

Description

Simulated data set (see data-raw/generate-data-densityratio.R) with five variables that are used in the examples.

Format

A data frame with 1000 rows and 5 columns:

- x1 Categorical variable with three categories, 'A', 'B' and 'C'
- x2 Categorical variable with two categories, 'G1' and 'G2'
- x3 Continuous variable (normally distributed given x1 and x2)
- **x4** Continuous variable (normally distributed given x3)
- **x5** Continuous variable (mixture of two normally distributed variables)

numerator_small

numerator small

Description

Subset of the numerator_data with three variables and 50 observations

Format

A data frame with 50 rows and 3 columns:

- x1 Continuous variable (normally distributed given x1 and x2)
- **x2** Continuous variable (normally distributed given x3)
- **x3** Continuous variable (mixture of two normally distributed variables)

18 permute

permute

Single permutation

Description

Single permutation

Single permutation statistic of ulsif object

Single permutation statistic of kliep object

Single permutation statistic of kmm object

Single permutation statistic of 1hss object

Single permutation statistic of spectral object

Single permutation statistic of naivedensityratio object

Usage

```
permute(object, ...)
## S3 method for class 'ulsif'
permute(object, stacked, nnu, nde, ...)
## S3 method for class 'kliep'
permute(object, stacked, nnu, nde, min_pred = sqrt(.Machine$double.eps), ...)
## S3 method for class 'kmm'
permute(object, stacked, nnu, nde, ...)
## S3 method for class 'lhss'
permute(object, stacked, nnu, nde, ...)
## S3 method for class 'spectral'
permute(object, stacked, nnu, nde, ...)
## S3 method for class 'naivedensityratio'
permute(object, stacked, nnu, nde, min_pred, max_pred, ...)
```

Arguments

max_pred

object	naivedensityratio object
	Additional arguments to pass through to specific permute functions.
stacked	matrix with stacked numerator and denominator samples
nnu	Scalar with numerator sample size
nde	Scalar with denominator sample size
min_pred	Minimum value of the predicted density ratio

Maximum value of the predicted density ratio

plot_bivariate 19

Value

permutation statistic for a single permutation of the data permutation statistic for a single permutation of the data permutation statistic for a single permutation of the data permutation statistic for a single permutation of the data permutation statistic for a single permutation of the data permutation statistic for a single permutation of the data permutation statistic for a single permutation of the data

plot_bivariate

Densityratio in two-dimensional plot

Description

Plots a scatterplot of two variables, with densityratio mapped to the colour scale.

Usage

```
plot_bivariate(
    x,
    vars = NULL,
    samples = "both",
    grid = FALSE,
    logscale = TRUE,
    show.sample = FALSE,
    tol = 0.01,
    ...
)
```

Arguments

X	Density ratio object created with e.g., kliep(), ulsif(), or naive()
vars	Character vector of variable names for which all pairwise bivariate plots are created
samples	Character string indicating whether to plot the 'numerator', 'denominator', or 'both' samples. Default is 'both'.
grid	Logical indicating whether output should be a list of individual plots ("individual"), or one facetted plot with all variables ("assembled"). Defaults to "individual".
logscale	Logical indicating whether to plot the density ratio estimates on a log scale. Default is TRUE.
show.sample	Logical indicating whether to give different shapes to observations, depending on the sample they come from (numerator or denominator). Defaults to FALSE.

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Numeric indicating the tolerance: values below this value will be set to the tolerance value, for legibility of the plots

Additional arguments passed to the predict() function.

Value

Bivariate scatter plots of all combinations of variables in vars.

Examples

```
set.seed(123)
# Fit model
dr <- ulsif(numerator_small, denominator_small)</pre>
# Inspect model object
# Obtain summary of model object
summary(dr)
# Plot model object
plot(dr)
# Plot density ratio for each variable individually
plot_univariate(dr)
# Plot density ratio for each pair of variables
plot_bivariate(dr)
# Predict density ratio and inspect first 6 predictions
head(predict(dr))
# Fit model with custom parameters
ulsif(numerator_small, denominator_small, sigma = 2, lambda = 2)
```

plot_univariate

Scatter plot of density ratios and individual variables

Description

A scatter plot showing the relationship between estimated density ratios and individual variables.

Usage

```
plot_univariate(
    x,
    vars = NULL,
    samples = "both",
    logscale = TRUE,
    grid = FALSE,
    sample.facet = FALSE,
    nrow.panel = NULL,
    tol = 0.01,
    ...
)
```

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Arguments

X	Density ratio object created with e.g., kliep(), ulsif(), or naive()
vars	Character vector of variable names to be plotted.
samples	Character string indicating whether to plot the 'numerator', 'denominator', or 'both' samples. Default is 'both'.
logscale	Logical indicating whether to plot the density ratio estimates on a log scale. Default is TRUE.
grid	Logical indicating whether output should be a list of individual plots ("individual"), or one facetted plot with all variables ("assembled"). Defaults to "individual".
sample.facet	Logical indicating whether to facet the plot by sample, i.e, showing plots separate for each sample, and side to side. Defaults to FALSE.
nrow.panel	Integer indicating the number of rows in the assembled plot. If NULL, the number of rows is automatically calculated.
tol	Numeric indicating the tolerance: values below this value will be set to the tolerance value, for legibility of the plots
	Additional arguments passed to the predict() function.

Value

Scatter plot of density ratios and individual variables.

```
set.seed(123)
# Fit model
dr <- ulsif(numerator_small, denominator_small)</pre>
# Inspect model object
dr
# Obtain summary of model object
summary(dr)
# Plot model object
plot(dr)
# Plot density ratio for each variable individually
plot_univariate(dr)
# Plot density ratio for each pair of variables
plot_bivariate(dr)
# Predict density ratio and inspect first 6 predictions
head(predict(dr))
# Fit model with custom parameters
ulsif(numerator_small, denominator_small, sigma = 2, lambda = 2)
```

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predict.kliep

Obtain predicted density ratio values from a kliep object

Description

Obtain predicted density ratio values from a kliep object

Usage

```
## S3 method for class 'kliep'
predict(object, newdata = NULL, sigma = c("sigmaopt", "all"), ...)
```

Arguments

object A kliep object

newdata Optional matrix new data set to compute the density

sigma A scalar with the Gaussian kernel width

... Additional arguments to be passed to the function

Value

An array with predicted density ratio values from possibly new data, but otherwise the numerator samples.

See Also

```
predict, kliep
```

```
set.seed(123)
# Fit model
dr <- kliep(numerator_small, denominator_small)</pre>
# Inspect model object
# Obtain summary of model object
summary(dr)
# Plot model object
plot(dr)
# Plot density ratio for each variable individually
plot_univariate(dr)
# Plot density ratio for each pair of variables
plot_bivariate(dr)
# Predict density ratio and inspect first 6 predictions
head(predict(dr))
# Fit model with custom parameters
kliep(numerator_small, denominator_small,
      nsigma = 1, ncenters = 100, nfold = 10,
      epsilon = 10^{2:-5}, maxit = 500)
```

predict.kmm 23

predict.kmm

Obtain predicted density ratio values from a kmm object

Description

Obtain predicted density ratio values from a kmm object

Usage

```
## S3 method for class 'kmm'
predict(object, newdata = NULL, sigma = c("sigmaopt", "all"), ...)
```

Arguments

object A kmm object

newdata Optional matrix new data set to compute the density

sigma A scalar with the Gaussian kernel width

... Additional arguments to be passed to the function

Value

An array with predicted density ratio values from possibly new data, but otherwise the numerator samples.

See Also

```
predict, kmm
```

```
set.seed(123)
# Fit model
dr <- kmm(numerator_small, denominator_small)</pre>
# Inspect model object
dr
# Obtain summary of model object
summary(dr)
# Plot model object
plot(dr)
# Plot density ratio for each variable individually
plot_univariate(dr)
# Plot density ratio for each pair of variables
plot_bivariate(dr)
# Predict density ratio and inspect first 6 predictions
head(predict(dr))
# Fit model with custom parameters
kmm(numerator_small, denominator_small,
   nsigma = 5, ncenters = 100, nfold = 10,
```

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```
constrained = TRUE)
```

predict.lhss

Obtain predicted density ratio values from a 1hss object

Description

Obtain predicted density ratio values from a 1hss object

Usage

```
## $3 method for class 'lhss'
predict(
  object,
  newdata = NULL,
  sigma = c("sigmaopt", "all"),
  lambda = c("lambdaopt", "all"),
  ...
)
```

Arguments

```
object A lhss object

newdata Optional matrix new data set to compute the density
sigma A scalar with the Gaussian kernel width
lambda A scalar with the regularization parameter
... Additional arguments to be passed to the function
```

Value

An array with predicted density ratio values from possibly new data, but otherwise the numerator samples.

See Also

```
predict, lhss
```

predict.naivedensityratio 25

```
summary(dr)
# Plot model object
plot(dr)
# Plot density ratio for each variable individually
plot_univariate(dr)
# Plot density ratio for each pair of variables
plot_bivariate(dr)
# Predict density ratio and inspect first 6 predictions
head(predict(dr))
```

```
predict.naivedensityratio
```

 ${\it Obtain predicted density ratio values from a \ {\it naivedensityratio} \ object}$

Description

Obtain predicted density ratio values from a naivedensityratio object

Usage

```
## S3 method for class 'naivedensityratio'
predict(object, newdata = NULL, log = FALSE, tol = 1e-06, ...)
```

Arguments

object	A naive object
newdata	Optional matrix new data set to compute the density
log	A logical indicating whether to return the log of the density ratio
tol	Minimal density value to avoid numerical issues
	Additional arguments to be passed to the function

Value

An array with predicted density ratio values from possibly new data, but otherwise the numerator samples.

```
predict, naive
```

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Examples

```
set.seed(123)
# Fit model
dr <- naive(numerator_small, denominator_small)</pre>
# Inspect model object
# Obtain summary of model object
summary(dr)
# Plot model object
plot(dr)
# Plot density ratio for each variable individually
plot_univariate(dr)
# Plot density ratio for each pair of variables
plot_bivariate(dr)
# Predict density ratio and inspect first 6 predictions
head(predict(dr))
# Fit model with custom parameters
naive(numerator_small, denominator_small, m=2, kernel="epanechnikov")
```

predict.spectral

Obtain predicted density ratio values from a spectral object

Description

Obtain predicted density ratio values from a spectral object

Usage

```
## S3 method for class 'spectral'
predict(
  object,
  newdata = NULL,
  sigma = c("sigmaopt", "all"),
  m = c("opt", "all"),
  ...
)
```

Arguments

object	A spectral object
newdata	Optional matrix new data set to compute the density
sigma	A scalar with the Gaussian kernel width
m	integer indicating the dimension of the eigenvector expansion
	Additional arguments to be passed to the function

predict.ulsif 27

Value

An array with predicted density ratio values from possibly new data, but otherwise the numerator samples.

See Also

```
predict, spectral
```

predict.ulsif

Obtain predicted density ratio values from a ulsif object

Description

Obtain predicted density ratio values from a ulsif object

Usage

```
## $3 method for class 'ulsif'
predict(
  object,
  newdata = NULL,
  sigma = c("sigmaopt", "all"),
  lambda = c("lambdaopt", "all"),
  ...
)
```

Arguments

object A ulsif object

newdata Optional matrix new data set to compute the density
sigma A scalar with the Gaussian kernel width

lambda A scalar with the regularization parameter

Additional arguments to be passed to the function

Value

An array with predicted density ratio values from possibly new data, but otherwise the numerator samples.

```
predict, ulsif
```

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Examples

```
set.seed(123)
# Fit model
dr <- ulsif(numerator_small, denominator_small)</pre>
# Inspect model object
# Obtain summary of model object
summary(dr)
# Plot model object
plot(dr)
# Plot density ratio for each variable individually
plot_univariate(dr)
# Plot density ratio for each pair of variables
plot_bivariate(dr)
# Predict density ratio and inspect first 6 predictions
head(predict(dr))
# Fit model with custom parameters
ulsif(numerator_small, denominator_small, sigma = 2, lambda = 2)
```

print.kliep

Print a kliep object

Description

Print a kliep object

Usage

```
## S3 method for class 'kliep'
print(x, digits = max(3L, getOption("digits") - 3L), ...)
```

Arguments

x Object of class kliep.digits Number of digits to use when printing the output.... further arguments on how to format the number of digits.

Value

invisble The inputted kliep object.

```
print, kliep
```

print.kmm 29

Examples

```
set.seed(123)
# Fit model
dr <- kliep(numerator_small, denominator_small)</pre>
# Inspect model object
# Obtain summary of model object
summary(dr)
# Plot model object
plot(dr)
# Plot density ratio for each variable individually
plot_univariate(dr)
# Plot density ratio for each pair of variables
plot_bivariate(dr)
# Predict density ratio and inspect first 6 predictions
head(predict(dr))
# Fit model with custom parameters
kliep(numerator_small, denominator_small,
      nsigma = 1, ncenters = 100, nfold = 10,
      epsilon = 10^{2:-5}, maxit = 500)
```

print.kmm

Print a kmm object

Description

Print a kmm object

Usage

```
## S3 method for class 'kmm'
print(x, digits = max(3L, getOption("digits") - 3L), ...)
```

Arguments

x Object of class kmm.

digits Number of digits to use when printing the output.

... further arguments on how to format the number of digits.

Value

invisble The inputted $\ensuremath{\mathsf{kmm}}$ object.

```
print, kmm
```

print.lhss

Examples

```
set.seed(123)
# Fit model
dr <- kmm(numerator_small, denominator_small)</pre>
# Inspect model object
# Obtain summary of model object
summary(dr)
# Plot model object
plot(dr)
# Plot density ratio for each variable individually
plot_univariate(dr)
# Plot density ratio for each pair of variables
plot_bivariate(dr)
# Predict density ratio and inspect first 6 predictions
head(predict(dr))
# Fit model with custom parameters
kmm(numerator_small, denominator_small,
   nsigma = 5, ncenters = 100, nfold = 10,
   constrained = TRUE)
```

print.lhss

Print a 1hss object

Description

Print a 1hss object

Usage

```
## S3 method for class 'lhss'
print(x, digits = max(3L, getOption("digits") - 3L), ...)
```

Arguments

x Object of class 1hss.

digits Number of digits to use when printing the output.

... further arguments on how to format the number of digits.

Value

invisble The inputted 1hss object.

```
print, lhss
```

print.naivedensityratio 31

Examples

```
set.seed(123)
# Fit model (minimal example to limit computation time)
dr <- lhss(numerator_small, denominator_small,</pre>
           nsigma = 5, nlambda = 3, ncenters = 50, maxit = 100)
# Inspect model object
dr
# Obtain summary of model object
summary(dr)
# Plot model object
plot(dr)
# Plot density ratio for each variable individually
plot_univariate(dr)
# Plot density ratio for each pair of variables
plot_bivariate(dr)
# Predict density ratio and inspect first 6 predictions
head(predict(dr))
```

print.naivedensityratio

Print a naivedensityratio object

Description

Print a naivedensityratio object

Usage

```
## S3 method for class 'naivedensityratio'
print(x, digits = max(3L, getOption("digits") - 3L), ...)
```

Arguments

x Object of class naivesubspacedensityratio.digits Number of digits to use when printing the output.... further arguments on how to format the number of digits.

Value

invisble The inputted naivedensityratio object.

```
print, naive
```

32 print.spectral

Examples

```
set.seed(123)
# Fit model
dr <- naive(numerator_small, denominator_small)</pre>
# Inspect model object
# Obtain summary of model object
summary(dr)
# Plot model object
plot(dr)
# Plot density ratio for each variable individually
plot_univariate(dr)
# Plot density ratio for each pair of variables
plot_bivariate(dr)
# Predict density ratio and inspect first 6 predictions
head(predict(dr))
# Fit model with custom parameters
naive(numerator_small, denominator_small, m=2, kernel="epanechnikov")
```

print.spectral

Print a spectral object

Description

Print a spectral object

Usage

```
## S3 method for class 'spectral'
print(x, digits = max(3L, getOption("digits") - 3L), ...)
```

Arguments

x Object of class spectral.digits Number of digits to use when printing the output.

... further arguments on how to format the number of digits.

Value

invisble The inputted spectral object.

```
print, spectral
```

print.summary.kliep 33

Examples

```
set.seed(123)
# Fit model
dr <- spectral(numerator_small, denominator_small)</pre>
# Inspect model object
# Obtain summary of model object
summary(dr)
# Plot model object
plot(dr)
# Plot density ratio for each variable individually
plot_univariate(dr)
# Plot density ratio for each pair of variables
plot_bivariate(dr)
# Predict density ratio and inspect first 6 predictions
head(predict(dr))
# Fit model with custom parameters
spectral(numerator_small, denominator_small, sigma = 2)
```

print.summary.kliep Print a summary.kliep object

Description

Print a summary.kliep object

Usage

```
## S3 method for class 'summary.kliep'
print(x, digits = max(3L, getOption("digits") - 3L), ...)
```

Arguments

x Object of class summary.kliep.digits Number of digits to use when printing the output.... further arguments on how to format the number of digits.

Value

invisble The inputted summary.kliep object.

```
print, summary.kliep, kliep
```

34 print.summary.kmm

Examples

```
set.seed(123)
# Fit model
dr <- kliep(numerator_small, denominator_small)</pre>
# Inspect model object
# Obtain summary of model object
summary(dr)
# Plot model object
plot(dr)
# Plot density ratio for each variable individually
plot_univariate(dr)
# Plot density ratio for each pair of variables
plot_bivariate(dr)
# Predict density ratio and inspect first 6 predictions
head(predict(dr))
# Fit model with custom parameters
kliep(numerator_small, denominator_small,
      nsigma = 1, ncenters = 100, nfold = 10,
      epsilon = 10^{2:-5}, maxit = 500)
```

print.summary.kmm

Print a summary.kmm object

Description

Print a summary.kmm object

Usage

```
## S3 method for class 'summary.kmm'
print(x, digits = max(3L, getOption("digits") - 3L), ...)
```

Arguments

x Object of class summary.kmm.

digits Number of digits to use when printing the output.

... further arguments on how to format the number of digits.

Value

invisble The inputted summary.kmm object.

```
print, summary.kmm, kmm
```

print.summary.lhss 35

Examples

```
set.seed(123)
# Fit model
dr <- kmm(numerator_small, denominator_small)</pre>
# Inspect model object
# Obtain summary of model object
summary(dr)
# Plot model object
plot(dr)
# Plot density ratio for each variable individually
plot_univariate(dr)
# Plot density ratio for each pair of variables
plot_bivariate(dr)
# Predict density ratio and inspect first 6 predictions
head(predict(dr))
# Fit model with custom parameters
kmm(numerator_small, denominator_small,
   nsigma = 5, ncenters = 100, nfold = 10,
   constrained = TRUE)
```

print.summary.lhss

Print a summary. 1hss object

Description

Print a summary. 1hss object

Usage

```
## S3 method for class 'summary.lhss'
print(x, digits = max(3L, getOption("digits") - 3L), ...)
```

Arguments

x Object of class summary. lhss.digits Number of digits to use when printing the output.... further arguments on how to format the number of digits.

Value

invisble The inputted summary. lhss object.

```
print, summary.lhss, lhss
```

Examples

```
set.seed(123)
# Fit model (minimal example to limit computation time)
dr <- lhss(numerator_small, denominator_small,</pre>
           nsigma = 5, nlambda = 3, ncenters = 50, maxit = 100)
# Inspect model object
dr
# Obtain summary of model object
summary(dr)
# Plot model object
plot(dr)
# Plot density ratio for each variable individually
plot_univariate(dr)
# Plot density ratio for each pair of variables
plot_bivariate(dr)
# Predict density ratio and inspect first 6 predictions
head(predict(dr))
```

```
print.summary.naivedensityratio
```

Print a summary.naivedensityratio object

Description

Print a summary.naivedensityratio object

Usage

```
## S3 method for class 'summary.naivedensityratio'
print(x, digits = max(3L, getOption("digits") - 3L), ...)
```

Arguments

x Object of class summary.naivedensityratio.digits Number of digits to use when printing the output.... further arguments on how to format the number of digits.

Value

invisble The inputted summary.naivedensityratio object.

```
print, summary.naivedensityratio, naive
```

print.summary.spectral 37

Examples

```
set.seed(123)
# Fit model
dr <- naive(numerator_small, denominator_small)</pre>
# Inspect model object
# Obtain summary of model object
summary(dr)
# Plot model object
plot(dr)
# Plot density ratio for each variable individually
plot_univariate(dr)
# Plot density ratio for each pair of variables
plot_bivariate(dr)
# Predict density ratio and inspect first 6 predictions
head(predict(dr))
# Fit model with custom parameters
naive(numerator_small, denominator_small, m=2, kernel="epanechnikov")
```

print.summary.spectral

Print a summary.spectral object

Description

Print a summary. spectral object

Usage

```
## S3 method for class 'summary.spectral'
print(x, digits = max(3L, getOption("digits") - 3L), ...)
```

Arguments

x Object of class summary.spectral.

digits Number of digits to use when printing the output.

... further arguments on how to format the number of digits.

Value

invisble The inputted summary. spectral object.

See Also

```
print, summary.spectral, spectral
```

38 print.summary.ulsif

Examples

```
set.seed(123)
# Fit model
dr <- spectral(numerator_small, denominator_small)</pre>
# Inspect model object
# Obtain summary of model object
summary(dr)
# Plot model object
plot(dr)
# Plot density ratio for each variable individually
plot_univariate(dr)
# Plot density ratio for each pair of variables
plot_bivariate(dr)
# Predict density ratio and inspect first 6 predictions
head(predict(dr))
# Fit model with custom parameters
spectral(numerator_small, denominator_small, sigma = 2)
```

```
print.summary.ulsif Print a summary.ulsif object
```

Description

Print a summary.ulsif object

Usage

```
## S3 method for class 'summary.ulsif'
print(x, digits = max(3L, getOption("digits") - 3L), ...)
```

Arguments

x Object of class summary.ulsif.digits Number of digits to use when printing the output.further arguments on how to format the number of digits.

Value

invisble The inputted summary.ulsif object.

See Also

```
print, summary.ulsif, ulsif
```

print.ulsif 39

Examples

```
set.seed(123)
# Fit model
dr <- ulsif(numerator_small, denominator_small)</pre>
# Inspect model object
# Obtain summary of model object
summary(dr)
# Plot model object
plot(dr)
# Plot density ratio for each variable individually
plot_univariate(dr)
# Plot density ratio for each pair of variables
plot_bivariate(dr)
# Predict density ratio and inspect first 6 predictions
head(predict(dr))
# Fit model with custom parameters
ulsif(numerator_small, denominator_small, sigma = 2, lambda = 2)
```

print.ulsif

Print a ulsif object

Description

Print a ulsif object

Usage

```
## S3 method for class 'ulsif'
print(x, digits = max(3L, getOption("digits") - 3L), ...)
```

Arguments

x Object of class ulsif.digits Number of digits to use when printing the output.... further arguments on how to format the number of digits.

Value

invisble The inputted ulsif object.

See Also

```
print, ulsif
```

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Examples

```
set.seed(123)
# Fit model
dr <- ulsif(numerator_small, denominator_small)</pre>
# Inspect model object
# Obtain summary of model object
summary(dr)
# Plot model object
plot(dr)
# Plot density ratio for each variable individually
plot_univariate(dr)
# Plot density ratio for each pair of variables
plot_bivariate(dr)
# Predict density ratio and inspect first 6 predictions
head(predict(dr))
# Fit model with custom parameters
ulsif(numerator_small, denominator_small, sigma = 2, lambda = 2)
```

spectral

Spectral series based density ratio estimation

Description

Spectral series based density ratio estimation

Usage

```
spectral(
  df_numerator,
  df_denominator,
  m = NULL,
  scale = "numerator",
  nsigma = 10,
  sigma_quantile = NULL,
  sigma = NULL,
  ncenters = NULL,
  cv = TRUE,
  nfold = 10,
  parallel = FALSE,
  nthreads = NULL,
  progressbar = TRUE
)
```

Arguments

df_numerator data.frame with exclusively numeric variables with the numerator samples

spectral 41

df_denominator	data.frame with exclusively numeric variables with the denominator samples (must have the same variables as df_denominator)
m	Integer vector indicating the number of eigenvectors to use in the spectral series expansion. Defaults to 50 evenly spaced values between 1 and the number of denominator samples (or the largest number of samples that can be used as centers in the cross-validation scheme).
scale	"numerator", "denominator", or NULL, indicating whether to standardize each numeric variable according to the numerator means and standard deviations, the denominator means and standard deviations, or apply no standardization at all.
nsigma	Integer indicating the number of sigma values (bandwidth parameter of the Gaussian kernel gram matrix) to use in cross-validation.
sigma_quantile	NULL or numeric vector with probabilities to calculate the quantiles of the distance matrix to obtain sigma values. If NULL, nsigma values between 0.05 and 0.95 are used.
sigma	NULL or a scalar value to determine the bandwidth of the Gaussian kernel gram matrix. If NULL, nsigma values between 0.05 and 0.95 are used.
ncenters	integer If smaller than the number of denominator observations, an approximation to the eigenvector expansion based on only ncenters samples is performed, instead of the full expansion. This can be useful for large datasets. Defaults to NULL, such that all denominator samples are used.
CV	logical indicating whether to use cross-validation to determine the optimal sigma value and the optimal number of eigenvectors.
nfold	Integer indicating the number of folds to use in the cross-validation scheme. If cv is FALSE, this parameter is ignored.
parallel	logical indicating whether to use parallel processing in the cross-validation scheme.
nthreads	NULL or integer indicating the number of threads to use for parallel processing. If parallel processing is enabled, it defaults to the number of available threads minus one.
progressbar	Logical indicating whether or not to display a progressbar.

Value

spectral-object, containing all information to calculate the density ratio using optimal sigma and optimal spectral series expansion.

References

Izbicki, R., Lee, A. & Schafer, C. (2014). High-Dimensional Density Ratio Estimation with Extensions to Approximate Likelihood Computation. Proceedings of Machine Learning Research 33, 420-429. Available from https://proceedings.mlr.press/v33/izbicki14.html.

```
set.seed(123)
# Fit model
dr <- spectral(numerator_small, denominator_small)</pre>
```

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```
# Inspect model object
dr
# Obtain summary of model object
summary(dr)
# Plot model object
plot(dr)
# Plot density ratio for each variable individually
plot_univariate(dr)
# Plot density ratio for each pair of variables
plot_bivariate(dr)
# Predict density ratio and inspect first 6 predictions
head(predict(dr))
# Fit model with custom parameters
spectral(numerator_small, denominator_small, sigma = 2)
```

summary.kliep

Extract summary from kliep object, including two-sample significance test for homogeneity of the numerator and denominator samples

Description

Extract summary from kliep object, including two-sample significance test for homogeneity of the numerator and denominator samples

Usage

```
## S3 method for class 'kliep'
summary(
  object,
  test = FALSE,
  n_perm = 100,
  parallel = FALSE,
  cluster = NULL,
  min_pred = 1e-06,
  ...
)
```

Arguments

object	Object of class kliep
test	logical indicating whether to statistically test for homogeneity of the numerator and denominator samples.
n_perm	Scalar indicating number of permutation samples
parallel	logical indicating to run the permutation test in parallel
cluster	NULL or a cluster object created by makeCluster. If NULL and parallel = TRUE, it uses the number of available cores minus 1.
min_pred	Scalar indicating the minimum value for the predicted density ratio values (used in the divergence statistic) to avoid negative density ratio values.
	further arguments passed to or from other methods.

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Value

Summary of the fitted density ratio model

Examples

```
set.seed(123)
# Fit model
dr <- kliep(numerator_small, denominator_small)</pre>
# Inspect model object
dr
# Obtain summary of model object
summary(dr)
# Plot model object
plot(dr)
# Plot density ratio for each variable individually
plot_univariate(dr)
# Plot density ratio for each pair of variables
plot_bivariate(dr)
# Predict density ratio and inspect first 6 predictions
head(predict(dr))
# Fit model with custom parameters
kliep(numerator_small, denominator_small,
      nsigma = 1, ncenters = 100, nfold = 10,
      epsilon = 10^{2:-5}, maxit = 500)
```

summary.kmm

Extract summary from kmm object, including two-sample significance test for homogeneity of the numerator and denominator samples

Description

Extract summary from kmm object, including two-sample significance test for homogeneity of the numerator and denominator samples

Usage

```
## S3 method for class 'kmm'
summary(
  object,
  test = FALSE,
  n_perm = 100,
  parallel = FALSE,
  cluster = NULL,
  min_pred = 1e-06,
  ...
)
```

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Arguments

object	Object of class kmm
test	logical indicating whether to statistically test for homogeneity of the numerator and denominator samples.
n_perm	Scalar indicating number of permutation samples
parallel	logical indicating to run the permutation test in parallel
cluster	NULL or a cluster object created by makeCluster. If NULL and parallel = TRUE, it uses the number of available cores minus 1.
min_pred	Scalar indicating the minimum value for the predicted density ratio values (used in the divergence statistic) to avoid negative density ratio values.
	further arguments passed to or from other methods.

Value

Summary of the fitted density ratio model

Examples

```
set.seed(123)
# Fit model
dr <- kmm(numerator_small, denominator_small)</pre>
# Inspect model object
dr
# Obtain summary of model object
summary(dr)
# Plot model object
plot(dr)
# Plot density ratio for each variable individually
plot_univariate(dr)
# Plot density ratio for each pair of variables
plot_bivariate(dr)
# Predict density ratio and inspect first 6 predictions
head(predict(dr))
# Fit model with custom parameters
kmm(numerator_small, denominator_small,
    nsigma = 5, ncenters = 100, nfold = 10,
    constrained = TRUE)
```

summary.lhss Extract summary from lhss object, including two-sample significance test for homogeneity of the numerator and denominator samples

Description

Extract summary from 1hss object, including two-sample significance test for homogeneity of the numerator and denominator samples

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Usage

```
## S3 method for class 'lhss'
summary(
  object,
  test = FALSE,
  n_perm = 100,
  parallel = FALSE,
  cluster = NULL,
  ...
)
```

Arguments

object	Object of class 1hss
test	logical indicating whether to statistically test for homogeneity of the numerator and denominator samples.
n_perm	Scalar indicating number of permutation samples
parallel	logical indicating to run the permutation test in parallel
cluster	NULL or a cluster object created by makeCluster. If NULL and parallel = TRUE, it uses the number of available cores minus 1.
	further arguments passed to or from other methods.

Value

Summary of the fitted density ratio model

summary.naivedensityratio

Extract summary from naivedensityraito object, including twosample significance test for homogeneity of the numerator and denominator samples

Description

Extract summary from naivedensityraito object, including two-sample significance test for homogeneity of the numerator and denominator samples

Usage

```
## $3 method for class 'naivedensityratio'
summary(
  object,
  test = FALSE,
  n_perm = 100,
  parallel = FALSE,
  cluster = NULL,
  ...
)
```

Arguments

object	Object of class naivedensityratio
test	logical indicating whether to statistically test for homogeneity of the numerator and denominator samples.
n_perm	Scalar indicating number of permutation samples
parallel	logical indicating to run the permutation test in parallel
cluster	NULL or a cluster object created by makeCluster. If NULL and parallel = TRUE, it uses the number of available cores minus 1.
	further arguments passed to or from other methods.

Value

Summary of the fitted density ratio model

```
set.seed(123)
# Fit model
dr <- naive(numerator_small, denominator_small)
# Inspect model object
dr
# Obtain summary of model object</pre>
```

summary.spectral 47

```
summary(dr)
# Plot model object
plot(dr)
# Plot density ratio for each variable individually
plot_univariate(dr)
# Plot density ratio for each pair of variables
plot_bivariate(dr)
# Predict density ratio and inspect first 6 predictions
head(predict(dr))
# Fit model with custom parameters
naive(numerator_small, denominator_small, m=2, kernel="epanechnikov")
```

summary.spectral

Extract summary from spectral object, including two-sample significance test for homogeneity of the numerator and denominator samples

Description

Extract summary from spectral object, including two-sample significance test for homogeneity of the numerator and denominator samples

Usage

```
## $3 method for class 'spectral'
summary(
  object,
  test = FALSE,
  n_perm = 100,
  parallel = FALSE,
  cluster = NULL,
  ...
)
```

Arguments

object	Object of class spectral
test	logical indicating whether to statistically test for homogeneity of the numerator and denominator samples.
n_perm	Scalar indicating number of permutation samples
parallel	logical indicating to run the permutation test in parallel
cluster	NULL or a cluster object created by makeCluster. If NULL and parallel = TRUE, it uses the number of available cores minus 1.
	further arguments passed to or from other methods.

Value

Summary of the fitted density ratio model

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Examples

```
set.seed(123)
# Fit model
dr <- spectral(numerator_small, denominator_small)</pre>
# Inspect model object
# Obtain summary of model object
summary(dr)
# Plot model object
plot(dr)
# Plot density ratio for each variable individually
plot_univariate(dr)
# Plot density ratio for each pair of variables
plot_bivariate(dr)
# Predict density ratio and inspect first 6 predictions
head(predict(dr))
# Fit model with custom parameters
spectral(numerator_small, denominator_small, sigma = 2)
```

summary.ulsif

Extract summary from ulsif object, including two-sample significance test for homogeneity of the numerator and denominator samples

Description

Extract summary from ulsif object, including two-sample significance test for homogeneity of the numerator and denominator samples

Usage

```
## $3 method for class 'ulsif'
summary(
  object,
  test = FALSE,
  n_perm = 100,
  parallel = FALSE,
  cluster = NULL,
  ...
)
```

Arguments

object Object of class ulsif

test logical indicating whether to statistically test for homogeneity of the numerator

and denominator samples.

n_perm Scalar indicating number of permutation samples

parallel logical indicating to run the permutation test in parallel

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cluster NULL or a cluster object created by makeCluster. If NULL and parallel = TRUE, it uses the number of available cores minus 1.

... further arguments passed to or from other methods.

Value

Summary of the fitted density ratio model

Examples

```
set.seed(123)
# Fit model
dr <- ulsif(numerator_small, denominator_small)</pre>
# Inspect model object
# Obtain summary of model object
summary(dr)
# Plot model object
plot(dr)
# Plot density ratio for each variable individually
plot_univariate(dr)
# Plot density ratio for each pair of variables
plot_bivariate(dr)
# Predict density ratio and inspect first 6 predictions
head(predict(dr))
# Fit model with custom parameters
ulsif(numerator_small, denominator_small, sigma = 2, lambda = 2)
```

ulsif

Unconstrained least-squares importance fitting

Description

Unconstrained least-squares importance fitting

Usage

```
ulsif(
  df_numerator,
  df_denominator,
  intercept = TRUE,
  scale = "numerator",
  nsigma = 10,
  sigma_quantile = NULL,
  sigma = NULL,
  nlambda = 20,
  lambda = NULL,
  ncenters = 200,
```

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```
centers = NULL,
parallel = FALSE,
nthreads = NULL,
progressbar = TRUE)
```

Arguments

df_numerator	data.frame with exclusively numeric variables with the numerator samples
df_denominator	data.frame with exclusively numeric variables with the denominator samples (must have the same variables as df_denominator)
intercept	logical Indicating whether to include an intercept term in the model. Defaults to TRUE.
scale	"numerator", "denominator", or NULL, indicating whether to standardize each numeric variable according to the numerator means and standard deviations, the denominator means and standard deviations, or apply no standardization at all.
nsigma	Integer indicating the number of sigma values (bandwidth parameter of the Gaussian kernel gram matrix) to use in cross-validation.
sigma_quantile	NULL or numeric vector with probabilities to calculate the quantiles of the distance matrix to obtain sigma values. If NULL, nsigma values between 0.05 and 0.95 are used.
sigma	NULL or a scalar value to determine the bandwidth of the Gaussian kernel gram matrix. If NULL, nsigma values between 0.05 and 0.95 are used.
nlambda	Integer indicating the number of lambda values (regularization parameter), by default, lambda is set to 10^seq(3, -3, length.out = nlambda).
lambda	NULL or numeric vector indicating the lambda values to use in cross-validation
ncenters	Maximum number of Gaussian centers in the kernel gram matrix. Defaults to all numerator samples.
centers	NULL or numeric matrix with the same dimensions as the data, indicating the centers for the Gaussian kernel gram matrix.
parallel	$logical\ indicating\ whether\ to\ use\ parallel\ processing\ in\ the\ cross-validation\ scheme.$
nthreads	NULL or integer indicating the number of threads to use for parallel processing. If parallel processing is enabled, it defaults to the number of available threads minus one.
progressbar	Logical indicating whether or not to display a progressbar.

Value

ulsif-object, containing all information to calculate the density ratio using optimal sigma and optimal weights.

References

Kanamori, T., Hido, S., & Sugiyama, M. (2009). A least-squares approach to direct importance estimation. Journal of Machine Learning Research, 10, 1391-1445. Available from https://jmlr.org/papers/v10/kanamori09a.html

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```
set.seed(123)
# Fit model
dr <- ulsif(numerator_small, denominator_small)</pre>
# Inspect model object
# Obtain summary of model object
summary(dr)
# Plot model object
plot(dr)
# Plot density ratio for each variable individually
plot_univariate(dr)
# Plot density ratio for each pair of variables
plot_bivariate(dr)
# Predict density ratio and inspect first 6 predictions
head(predict(dr))
# Fit model with custom parameters
ulsif(numerator_small, denominator_small, sigma = 2, lambda = 2)
```

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