

Package ‘ks’

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Description Kernel smoothers for univariate and multivariate data, including densities, density derivatives, cumulative distributions, clustering, classification, density ridges, significant modal regions, and two-sample hypothesis tests. Chacon & Duong (2018) <doi:10.1201/9780429485572>.

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ks-package

ks

Description

Kernel smoothing for data from 1- to 6-dimensions.

Details

There are three main types of functions in this package:

- computing kernel estimators - these function names begin with ‘k’
- computing bandwidth selectors - these begin with ‘h’ (1-d) or ‘H’ (>1-d)
- displaying kernel estimators - these begin with ‘plot’.

The kernel used throughout is the normal (Gaussian) kernel K . For 1-d data, the bandwidth h is the standard deviation of the normal kernel, whereas for multivariate data, the bandwidth matrix \mathbf{H} is the variance matrix.

–For kernel density estimation, `kde` computes

$$\hat{f}(\mathbf{x}) = n^{-1} \sum_{i=1}^n K_{\mathbf{H}}(\mathbf{x} - \mathbf{X}_i).$$

The bandwidth matrix \mathbf{H} is a matrix of smoothing parameters and its choice is crucial for the performance of kernel estimators. For display, its `plot` method calls `plot.kde`.

–For kernel density estimation, there are several varieties of bandwidth selectors

- plug-in `hpi` (1-d); `Hpi`, `Hpi.diag` (2- to 6-d)
- least squares (or unbiased) cross validation (LSCV or UCV) `hlscv` (1-d); `Hlscv`, `Hlscv.diag` (2- to 6-d)
- biased cross validation (BCV) `Hbcv`, `Hbcv.diag` (2- to 6-d)
- smoothed cross validation (SCV) `hscv` (1-d); `Hscv`, `Hscv.diag` (2- to 6-d)
- normal scale `hns` (1-d); `Hns` (2- to 6-d).

–For kernel density support estimation, the main function is `ksupp` which is (the convex hull of)

$$\{\mathbf{x} : \hat{f}(\mathbf{x}) > \tau\}$$

for a suitable level τ . This is closely related to the τ -level set of \hat{f} .

–For truncated kernel density estimation, the main function is `kde.truncate`

$$\hat{f}(\mathbf{x}) \mathbf{1}\{\mathbf{x} \in \Omega\} / \int_{\Omega} \hat{f}(\mathbf{x}) d\mathbf{x}$$

for a bounded data support Ω . The standard density estimate \hat{f} is truncated and rescaled to give unit integral over Ω . Its `plot` method calls `plot.kde`.

–For boundary kernel density estimation where the kernel function is modified explicitly in the boundary region, the main function is `kde.boundary`

$$n^{-1} \sum_{i=1}^n K_{\mathbf{H}}^*(\mathbf{x} - \mathbf{X}_i)$$

for a boundary kernel K^* . Its `plot` method calls `plot.kde`.

–For variable kernel density estimation where the bandwidth is not a constant matrix, the main functions are `kde.balloon`

$$\hat{f}_{\text{ball}}(\mathbf{x}) = n^{-1} \sum_{i=1}^n K_{\mathbf{H}(\mathbf{x})}(\mathbf{x} - \mathbf{X}_i)$$

and `kde.sp`

$$\hat{f}_{\text{SP}}(\mathbf{x}) = n^{-1} \sum_{i=1}^n K_{\mathbf{H}(\mathbf{X}_i)}(\mathbf{x} - \mathbf{X}_i).$$

For the balloon estimation \hat{f}_{ball} the bandwidth varies with the estimation point \mathbf{x} , whereas for the sample point estimation \hat{f}_{SP} the bandwidth varies with the data point $\mathbf{X}_i, i = 1, \dots, n$. Their `plot` methods call `plot.kde`. The bandwidth selectors for `kde.balloon` are based on the normal scale bandwidth `Hns(,deriv.order=2)` via the MSE minimal formula, and for `kde.SP` on `Hns(,deriv.order=4)` via the Abramson formula.

–For kernel density derivative estimation, the main function is `kdde`

$$D^{\otimes r} \hat{f}(\mathbf{x}) = n^{-1} \sum_{i=1}^n D^{\otimes r} K_{\mathbf{H}}(\mathbf{x} - \mathbf{X}_i).$$

The bandwidth selectors are a modified subset of those for `kde`, i.e. `Hlscv`, `Hns`, `Hpi`, `Hscv` with `deriv.order>0`. Its `plot` method is `plot.kdde` for plotting each partial derivative singly.

–For kernel summary curvature estimation, the main function is `kcurv`

$$\hat{s}(\mathbf{x}) = -\mathbf{1}\{D^2 \hat{f}(\mathbf{x}) < 0\} \text{abs}(|D^2 \hat{f}(\mathbf{x})|)$$

where $D^2 \hat{f}(\mathbf{x})$ is the kernel Hessian matrix estimate. It has the same structure as a kernel density estimate so its `plot` method calls `plot.kde`.

–For kernel discriminant analysis, the main function is `kda` which computes density estimates for each the groups in the training data, and the discriminant surface. Its `plot` method is `plot.kda`. The wrapper function `hkda`, `Hkda` computes bandwidths for each group in the training data for `kde`, e.g. `hpi`, `Hpi`.

–For kernel functional estimation, the main function is `kfe` which computes the r -th order integrated density functional

$$\hat{\psi}_r = n^{-2} \sum_{i=1}^n \sum_{j=1}^n D^{\otimes r} K_{\mathbf{H}}(\mathbf{X}_i - \mathbf{X}_j).$$

The plug-in selectors are `hpi.kfe` (1-d), `Hpi.kfe` (2- to 6-d). Kernel functional estimates are usually not required to be computed directly by the user, but only within other functions in the package.

–For kernel-based 2-sample testing, the main function is `kde.test` which computes the integrated L_2 distance between the two density estimates as the test statistic, comprising a linear combination of 0-th order kernel functional estimates:

$$\hat{T} = \hat{\psi}_{0,1} + \hat{\psi}_{0,2} - (\hat{\psi}_{0,12} + \hat{\psi}_{0,21}),$$

and the corresponding p-value. The ψ are zero order kernel functional estimates with the subscripts indicating that 1 = sample 1 only, 2 = sample 2 only, and 12, 21 = samples 1 and 2. The bandwidth selectors are `hpi.kfe`, `Hpi.kfe` with `deriv.order=0`.

–For kernel-based local 2-sample testing, the main function is `kde.local.test` which computes the squared distance between the two density estimates as the test statistic

$$\hat{U}(\mathbf{x}) = [\hat{f}_1(\mathbf{x}) - \hat{f}_2(\mathbf{x})]^2$$

and the corresponding local p-values. The bandwidth selectors are those used with `kde`, e.g. `hpi`, `Hpi`.

–For kernel cumulative distribution function estimation, the main function is `kcde`

$$\hat{F}(\mathbf{x}) = n^{-1} \sum_{i=1}^n \mathcal{K}_{\mathbf{H}}(\mathbf{x} - \mathbf{X}_i)$$

where \mathcal{K} is the integrated kernel. The bandwidth selectors are `hpi.kcde`, `Hpi.kcde`. Its plot method is `plot.kcde`. There exist analogous functions for the survival function \hat{F} .

–For kernel estimation of a ROC (receiver operating characteristic) curve to compare two samples from \hat{F}_1, \hat{F}_2 , the main function is `kroc`

$$\{\hat{F}_{\hat{Y}_1}(z), \hat{F}_{\hat{Y}_2}(z)\}$$

based on the cumulative distribution functions of $\hat{Y}_j = \hat{F}_1^{-1}(\mathbf{X}_j), j = 1, 2$.

The bandwidth selectors are those used with `kcde`, e.g. `hpi.kcde`, `Hpi.kcde` for $\hat{F}_{\hat{Y}_j}, \hat{F}_1$. Its plot method is `plot.kroc`.

–For kernel estimation of a copula, the main function is `kcopula`

$$\hat{C}(\mathbf{z}) = \hat{F}(\hat{F}_1^{-1}(z_1), \dots, \hat{F}_d^{-1}(z_d))$$

where $\hat{F}_j^{-1}(z_j)$ is the z_j -th quantile of the j -th marginal distribution \hat{F}_j . The bandwidth selectors are those used with `kcde` for \hat{F}, \hat{F}_j . Its plot method is `plot.kcde`.

–For kernel mean shift clustering, the main function is `kms`. The mean shift recurrence relation of the candidate point \mathbf{x}

$$\mathbf{x}_{j+1} = \mathbf{x}_j + \mathbf{HD}\hat{f}(\mathbf{x}_j)/\hat{f}(\mathbf{x}_j),$$

where $j \geq 0$ and $\mathbf{x}_0 = \mathbf{x}$, is iterated until \mathbf{x} converges to its local mode in the density estimate \hat{f} by following the density gradient ascent paths. This mode determines the cluster label for \mathbf{x} . The bandwidth selectors are those used with `kdde`(, `deriv.order=1`).

–For kernel density ridge estimation, the main function is `kdr`. The kernel density ridge recurrence relation of the candidate point \mathbf{x}

$$\mathbf{x}_{j+1} = \mathbf{x}_j + \mathbf{U}_{(d-1)}(\mathbf{x}_j)\mathbf{U}_{(d-1)}(\mathbf{x}_j)^T \mathbf{HD}\hat{f}(\mathbf{x}_j)/\hat{f}(\mathbf{x}_j),$$

where $j \geq 0$, $\mathbf{x}_0 = \mathbf{x}$ and $\mathbf{U}_{(d-1)}$ is the 1-dimensional projected density gradient, is iterated until \mathbf{x} converges to the ridge in the density estimate. The bandwidth selectors are those used with `kdde(,deriv.order=2)`.

– For kernel feature significance, the main function is `kfs`. The hypothesis test at a point \mathbf{x} is $H_0(\mathbf{x}) : \mathbf{H}f(\mathbf{x}) < 0$, i.e. the density Hessian matrix $\mathbf{H}f(\mathbf{x})$ is negative definite. The test statistic is

$$W(\mathbf{x}) = \|\mathbf{S}(\mathbf{x})^{-1/2} \text{vech } \mathbf{H}\hat{f}(\mathbf{x})\|^2$$

where $\mathbf{H}\hat{f}$ is the Hessian estimate, `vech` is the vector-half operator, and \mathbf{S} is an estimate of the null variance. $W(\mathbf{x})$ is approximately χ^2 distributed with $d(d+1)/2$ degrees of freedom. If $H_0(\mathbf{x})$ is rejected, then \mathbf{x} belongs to a significant modal region. The bandwidth selectors are those used with `kdde(,deriv.order=2)`. Its plot method is `plot.kfs`.

– For deconvolution density estimation, the main function is `kdcde`. A weighted kernel density estimation with the contaminated data $\mathbf{W}_1, \dots, \mathbf{W}_n$,

$$\hat{f}_w(\mathbf{x}) = n^{-1} \sum_{i=1}^n \alpha_i K_{\mathbf{H}}(\mathbf{x} - \mathbf{W}_i),$$

is utilised, where the weights $\alpha_1, \dots, \alpha_n$ are chosen via a quadratic optimisation involving the error variance and the regularisation parameter. The bandwidth selectors are those used with `kde`.

– Binned kernel estimation is an approximation to the exact kernel estimation and is available for $d=1, 2, 3, 4$. This makes kernel estimators feasible for large samples.

– For an overview of this package with 2-d density estimation, see `vignette("kde")`.

– For `ks` $\geq 1.11.1$, the `misc3d` and `rgl` (3-d plot), `OceanView` (quiver plot), `oz` (Australian map) packages have been moved from Depends to Suggests. This was done to allow `ks` to be installed on systems where these latter graphical-based packages can't be installed.

Author(s)

Tarn Duong for most of the package. M. P. Wand for the binned estimation, univariate plug-in selector and univariate density derivative estimator code. J. E. Chacon for the unconstrained pilot functional estimation and fast implementation of derivative-based estimation code. A. and J. Gramacki for the binned estimation for unconstrained bandwidth matrices.

References

- Bowman, A. & Azzalini, A. (1997) *Applied Smoothing Techniques for Data Analysis*. Oxford University Press, Oxford.
- Chacon, J.E. & Duong, T. (2018) *Multivariate Kernel Smoothing and Its Applications*. Chapman & Hall/CRC. To appear.
- Duong, T. (2004) *Bandwidth Matrices for Multivariate Kernel Density Estimation*. Ph.D. Thesis, University of Western Australia.
- Scott, D.W. (1992) *Multivariate Density Estimation: Theory, Practice, and Visualization*. John Wiley & Sons, New York.
- Silverman, B. (1986) *Density Estimation for Statistics and Data Analysis*. Chapman & Hall/CRC, London.
- Simonoff, J. S. (1996) *Smoothing Methods in Statistics*. Springer-Verlag, New York.
- Wand, M.P. & Jones, M.C. (1995) *Kernel Smoothing*. Chapman & Hall/CRC, London.

See Also

feature, sm, KernSmooth

air

Air quality measurements in an underground train station

Description

This data set contains the hourly mean air quality measurements from 01 January 2013 to 31 December 2016 in the Chatelet underground train station in the Paris metro.

Usage

```
data(air)
```

Format

A matrix with 35039 rows and 8 columns. Each row corresponds to an hourly measurement. The first column is the date (yyyy-mm-dd), the second is the time (hh:mm), the third is the nitric oxide NO concentration (g/m³), the fourth is the nitrogen dioxide NO₂ concentration (g/m³), the fifth is the concentration of particulate matter less than 10 microns PM₁₀ (ppm), the sixth is the carbon dioxide concentration CO₂ (g/m³), the seventh is the temperature (degrees Celsius), the eighth is the relative humidity (percentage).

Source

RATP (2016) Qualite de l'air mesuree dans la station Chatelet, <https://data.iledefrance.fr/explore/dataset/qualite-de-lair-mesuree-dans-la-station-chatelet>. Regie autonome des transports parisiens - Departement Developpement, Innovation et Territoires. Accessed 2017-09-27.

binning

Linear binning for multivariate data

Description

Linear binning for 1- to 4-dimensional data.

Usage

```
binning(x, H, h, bgridsize, xmin, xmax, supp=3.7, w, gridtype="linear")
```

Arguments

x	matrix of data values
H, h	bandwidth matrix, scalar bandwidth
xmin, xmax	vector of minimum/maximum values for grid
supp	effective support for standard normal is [-supp, supp]
bgridsize	vector of binning grid sizes
w	vector of weights. Default is a vector of all ones.
gridtype	not yet implemented

Details

As of **ks** 1.10.0, binning is available for unconstrained (non-diagonal) bandwidth matrices. Code is used courtesy of A. & J. Gramacki, and M.P. Wand. Default bgridsize are d=1: 401; d=2: rep(151, 2); d=3: rep(51, 3); d=4: rep(21, 4).

Value

Returns a list with 2 fields

counts	linear binning counts
eval.points	vector (d=1) or list (d>=2) of grid points in each dimension

References

Gramacki, A. & Gramacki, J. (2016) FFT-based fast computation of multivariate kernel estimators with unconstrained bandwidth matrices. *Journal of Computational & Graphical Statistics*, **26**, 459-462.

Wand, M.P. & Jones, M.C. (1995) *Kernel Smoothing*. Chapman & Hall. London.

Examples

```
data(unicef)
ubinned <- binning(x=unicef)
```

cardio

Foetal cardiotocograms

Description

This data set contains the cardiotocographic measurements from healthy, suspect and pathological foetuses.

Usage

```
data(cardio)
```


Format

A matrix with 2126 rows and 8 columns. Each row corresponds to a foetal cardiocotogram. The class label for the foetal state is the last column: N = normal, S = suspect, P = pathological. Details for all variables are found in the link below.

Source

Lichman, M. (2013) UCI machine learning repository, <http://archive.ics.uci.edu/ml/datasets/Cardiotocography>. University of California, Irvine, School of Information and Computer Sciences. Accessed 2017-05-18.

contour	<i>Contours functions</i>
---------	---------------------------

Description

Contour levels and sizes.

Usage

```
contourLevels(x, ...)
## S3 method for class 'kde'
contourLevels(x, prob, cont, nlevels=5, approx=TRUE, ...)
## S3 method for class 'kda'
contourLevels(x, prob, cont, nlevels=5, approx=TRUE, ...)

contourSizes(x, abs.cont, cont=c(25,50,75), approx=TRUE)
```

Arguments

x	an object of class kde or kda
prob	vector of probabilities corresponding to highest density regions
cont	vector of percentages which correspond to the complement of prob
abs.cont	vector of absolute contour levels
nlevels	number of pretty contour levels
approx	flag to compute approximate contour levels. Default is TRUE.
...	other parameters

Details

–For `contourLevels`, the most straightforward is to specify `prob`. Heights of the corresponding highest density region with probability `prob` are computed. The `cont` parameter here is consistent with `cont` parameter from `plot.kde` and `plot.kda` i.e. `cont=(1-prob)*100%`. If both `prob` and `cont` are missing then a pretty set of `nlevels` contours are computed.

–For `contourSizes`, the length, area, volume etc. are approximated by Riemann sums. These are rough approximations and depend highly on the estimation grid, and so should be interpreted carefully.

If `approx=FALSE`, then the exact KDE is computed. Otherwise it is interpolated from an existing KDE grid. This can dramatically reduce computation time for large data sets.

Value

–For `contourLevels`, for kde objects, returns vector of heights. For kda objects, returns a list of vectors, one for each training group.

–For `contourSizes`, an approximation of the Lebesgue measure of level set, i.e. length (d=1), area (d=2), volume (d=3), hyper-volume (d>4).

See Also

[contour](#), [contourLines](#)

Examples

```
set.seed(8192)
x <- rmvnorm.mixt(n=1000, mus=c(0,0), Sigmas=diag(2), props=1)
fhat <- kde(x=x, binned=TRUE)
contourLevels(fhat, cont=c(75, 50, 25))
contourSizes(fhat, cont=25, approx=TRUE)
## compare to approx circle of radius=0.75 with area=1.77
```

grevillea

Geographical locations of grevillea plants

Description

This data set contains the geographical locations of the specimens of *Grevillea uncinulata*, more commonly known as the Hook leaf grevillea, which is an endemic floral species to south Western Australia. This region is one of the 25 ‘biodiversity hotspots’ which are ‘areas featuring exceptional concentrations of endemic species and experiencing exceptional loss of habitat’.

Usage

```
data(grevillea)
```

Format

A matrix with 222 rows and 2 columns. Each row corresponds to a observed plant. The first column is the longitude (decimal degrees), the second is the latitude (decimal degrees).

Source

CSIRO (2016) Atlas of Living Australia: *Grevillea uncinulata* Diels, <http://bie.ala.org.au/species/urn:lsid:biodiversity.org.au:apni.taxon:249319>. Commonwealth Scientific and Industrial Research Organisation. Accessed 2016-03-11.

Hbcv	<i>Biased cross-validation (BCV) bandwidth matrix selector for bivariate data</i>
------	---

Description

BCV bandwidth matrix for bivariate data.

Usage

```
Hbcv(x, whichbcv=1, Hstart, binned=FALSE, amise=FALSE, verbose=FALSE)
Hbcv.diag(x, whichbcv=1, Hstart, binned=FALSE, amise=FALSE, verbose=FALSE)
```

Arguments

x	matrix of data values
whichbcv	1 = BCV1, 2 = BCV2. See details below.
Hstart	initial bandwidth matrix, used in numerical optimisation
binned	flag for binned kernel estimation. Default is FALSE.
amise	flag to return the minimal BCV value. Default is FALSE.
verbose	flag to print out progress information. Default is FALSE.

Details

Use `Hbcv` for unconstrained bandwidth matrices and `Hbcv.diag` for diagonal bandwidth matrices. These selectors are only available for bivariate data. Two types of BCV criteria are considered here. They are known as BCV1 and BCV2, from Sain, Baggerly & Scott (1994) and only differ slightly. These BCV surfaces can have multiple minima and so it can be quite difficult to locate the most appropriate minimum. Some times, there can be no local minimum at all so there may be no finite BCV selector.

For details about the advanced options for `binned`, `Hstart`, see [Hpi](#).

Value

BCV bandwidth matrix. If `amise=TRUE` then the minimal BCV value is returned too.

References

Sain, S.R, Baggerly, K.A. & Scott, D.W. (1994) Cross-validation of multivariate densities. *Journal of the American Statistical Association*, **82**, 1131-1146.

See Also

[Hlscv](#), [Hpi](#), [Hscv](#)

Examples

```
data(unicef)
Hbcv(unicef)
Hbcv.diag(unicef)
```

histde	<i>Histogram density estimate</i>
--------	-----------------------------------

Description

Histogram density estimate for 1- and 2-dimensional data.

Usage

```
histde(x, binw, xmin, xmax, adj=0)

## S3 method for class 'histde'
predict(object, ..., x)
```

Arguments

x	matrix of data values
binw	(vector) of binwidths
xmin, xmax	vector of minimum/maximum values for grid
adj	displacement of default anchor point, in percentage of 1 bin
object	an object of class histde
...	other parameters

Details

If binw is missing, the default binwidth is $\hat{b}_i = 2 \cdot 3^{1/(d+2)} \pi^{d/(2d+4)} S_i n^{-1/(d+2)}$, the normal scale selector.

If xmin is missing then it defaults to the data minimum. If xmax is missing then it defaults to the data maximum.

Value

A histogram density estimate is an object of class `histde` which is a list with fields:

<code>x</code>	data points - same as input
<code>eval.points</code>	vector or list of points at which the estimate is evaluated
<code>estimate</code>	density estimate at <code>eval.points</code>
<code>binw</code>	(vector of) bandwidths
<code>nbin</code>	(vector of) number of bins
<code>names</code>	variable names

See Also

[plot.histde](#)

Examples

```
## positive data example
set.seed(8192)
x <- 2*rnorm(100)
fhat <- histde(x=x)
plot(fhat, col=3)
points(c(0.5, 1), predict(fhat, x=c(0.5, 1)))

## large data example on a non-default grid
set.seed(8192)
x <- rmvnorm.mixt(10000, mus=c(0,0), Sigmas=invvech(c(1,0.8,1)))
fhat <- histde(x=x, xmin=c(-5,-5), xmax=c(5,5))
plot(fhat)

## See other examples in ? plot.histde
```

Hlscv	<i>Least-squares cross-validation (LSCV) bandwidth matrix selector for multivariate data</i>
-------	--

Description

LSCV bandwidth for 1- to 6-dimensional data

Usage

```
Hlscv(x, Hstart, binned, bgridsize, amise=FALSE, deriv.order=0,
      verbose=FALSE, optim.fun="optim", trunc)
Hlscv.diag(x, Hstart, binned, bgridsize, amise=FALSE, deriv.order=0,
          verbose=FALSE, optim.fun="optim", trunc)
hlscv(x, binned=TRUE, bgridsize, amise=FALSE, deriv.order=0)
Hucv(...)
Hucv.diag(...)
hucv(...)
```

Arguments

<code>x</code>	vector or matrix of data values
<code>Hstart</code>	initial bandwidth matrix, used in numerical optimisation
<code>binned</code>	flag for binned kernel estimation
<code>bgridsize</code>	vector of binning grid sizes
<code>amise</code>	flag to return the minimal LSCV value. Default is FALSE.
<code>deriv.order</code>	derivative order
<code>verbose</code>	flag to print out progress information. Default is FALSE.
<code>optim.fun</code>	optimiser function: one of <code>nlm</code> or <code>optim</code>
<code>trunc</code>	parameter to control truncation for numerical optimisation. Default is 4 for <code>density.deriv>0</code> , otherwise no truncation. For details see below.
<code>...</code>	parameters as above

Details

`hlscv` is the univariate LSCV selector of Bowman (1984) and Rudemo (1982). `Hlscv` is a multivariate generalisation of this. Use `Hlscv` for unconstrained bandwidth matrices and `Hlscv.diag` for diagonal bandwidth matrices. `Hucv`, `Hucv.diag` and `hucv` are aliases with UCV (unbiased cross validation) instead of LSCV.

Truncation of the parameter space is usually required for the LSCV selector, for $r > 0$, to find a reasonable solution to the numerical optimisation. If a candidate matrix H is such that $\det(H)$ is not in $[1/\text{trunc}, \text{trunc}] * \det(H_0)$ or $\text{abs}(\text{LSCV}(H)) > \text{trunc} * \text{abs}(\text{LSCV}_0)$ then the $\text{LSCV}(H)$ is reset to LSCV_0 where $H_0 = H_{ns}(x)$ and $\text{LSCV}_0 = \text{LSCV}(H_0)$.

From `ks` 1.11.1 onwards, the default optimisation function is `optim.fun="optim"`.

For details about the advanced options for `binned`, `Hstart`, see [Hpi](#).

Value

LSCV bandwidth. If `amise=TRUE` then the minimal LSCV value is returned too.

References

Bowman, A. (1984) An alternative method of cross-validation for the smoothing of kernel density estimates. *Biometrika*, **71**, 353-360.

Rudemo, M. (1982) Empirical choice of histograms and kernel density estimators. *Scandinavian Journal of Statistics*, **9**, 65-78.

See Also

[Hbcv](#), [Hpi](#), [Hscv](#)

Examples

```
library(MASS)
data(forbes)
Hlscv(forbes)
hlscv(forbes$bp)
```

Hnm	<i>Normal mixture bandwidth</i>
-----	---------------------------------

Description

Normal mixture bandwidth.

Usage

```
Hnm(x, deriv.order=0, G=1:9, subset.ind, mise.flag=FALSE, verbose, ...)  
Hnm.diag(x, deriv.order=0, G=1:9, subset.ind, mise.flag=FALSE, verbose, ...)  
hnm(x, deriv.order=0, G=1:9, subset.ind, mise.flag=FALSE, verbose, ... )
```

Arguments

x	vector/matrix of data values
deriv.order	derivative order
G	range of number of mixture components
subset.ind	index vector of subset of x for fitting
mise.flag	flag to use MISE or AMISE minimisation. Default is FALSE.
verbose	flag to print out progress information. Default is FALSE.
...	other parameters for Mclust

Details

The normal mixture fit is provided by the `Mclust` function in the **mclust** package. `Hnm` is then `Hmise.mixt` (if `mise.flag=TRUE`) or `Hamise.mixt` (if `mise.flag=FALSE`) with these fitted normal mixture parameters. Likewise for `Hnm.diag`, `hnm`.

Value

Normal mixture bandwidth. If `mise=TRUE` then the minimal MISE value is returned too.

References

Cwik, J. & Koronacki, J. (1997). A combined adaptive-mixtures/plug-in estimator of multivariate probability densities. *Computational Statistics and Data Analysis*, **26**, 199-218.

See Also

[Hmise.mixt](#), [Hamise.mixt](#)

Examples

```
library(MASS)  
data(forbes)  
Hnm(forbes)
```

Hns	<i>Normal scale bandwidth</i>
-----	-------------------------------

Description

Normal scale bandwidth.

Usage

```
Hns(x, deriv.order=0)
Hns.diag(x)
hns(x, deriv.order=0)
Hns.kcde(x)
hns.kcde(x)
```

Arguments

x	vector/matrix of data values
deriv.order	derivative order

Details

Hns is equal to $(4/(n*(d+2*r+2)))^{2/(d+2*r+4)}*var(x)$, n = sample size, d = dimension of data, r = derivative order. hns is the analogue of Hns for 1-d data. These can be used for density (derivative) estimators [kde](#), [kdde](#). The equivalents for distribution estimators [kcde](#) are Hns.kcde and hns.cde.

Value

Normal scale bandwidth.

References

Chacon J.E., Duong, T. & Wand, M.P. (2011). Asymptotics for general multivariate kernel density derivative estimators. *Statistica Sinica*, **21**, 807-840.

Examples

```
library(MASS)
data(forbes)
Hns(forbes, deriv.order=2)
hns(forbes$bp, deriv.order=2)
```

Hpi *Plug-in bandwidth selector*

Description

Plug-in bandwidth for for 1- to 6-dimensional data.

Usage

```
Hpi(x, nstage=2, pilot, pre="sphere", Hstart, binned, bgridsize,
    amise=FALSE, deriv.order=0, verbose=FALSE, optim.fun="optim")
Hpi.diag(x, nstage=2, pilot, pre="scale", Hstart, binned, bgridsize,
    amise=FALSE, deriv.order=0, verbose=FALSE, optim.fun="optim")
hpi(x, nstage=2, binned=TRUE, bgridsize, deriv.order=0)
```

Arguments

x	vector or matrix of data values
nstage	number of stages in the plug-in bandwidth selector (1 or 2)
pilot	"amse" = AMSE pilot bandwidths "samse" = single SAMSE pilot bandwidth "unconstr" = single unconstrained pilot bandwidth "dscalar" = single pilot bandwidth for deriv.order >= 0 "dunconstr" = single unconstrained pilot bandwidth for deriv.order >= 0
pre	"scale" = pre.scale , "sphere" = pre.sphere
Hstart	initial bandwidth matrix, used in numerical optimisation
binned	flag for binned kernel estimation
bgridsize	vector of binning grid sizes
amise	flag to return the minimal scaled PI value
deriv.order	derivative order
verbose	flag to print out progress information. Default is FALSE.
optim.fun	optimiser function: one of nlm or optim

Details

`hpi(, deriv.order=0)` is the univariate plug-in selector of Wand & Jones (1994), i.e. it is exactly the same as **KernSmooth**'s `dpik`. For `deriv.order>0`, the formula is taken from Wand & Jones (1995). `Hpi` is a multivariate generalisation of this. Use `Hpi` for unconstrained bandwidth matrices and `Hpi.diag` for diagonal bandwidth matrices.

The default pilot is "samse" for `d=2,r=0`, and "dscalar" otherwise. For AMSE pilot bandwidths, see Wand & Jones (1994). For SAMSE pilot bandwidths, see Duong & Hazelton (2003). The latter is a modification of the former, in order to remove any possible problems with non-positive definiteness. Unconstrained and higher order derivative pilot bandwidths are from Chacon & Duong (2010).

For $d=1, 2, 3, 4$ and `binned=TRUE`, estimates are computed over a binning grid defined by `bgridsize`. Otherwise it's computed exactly. If `Hstart` is not given then it defaults to `Hns(x)`.

From `ks 1.11.1` onwards, the default optimisation function is `optim.fun="optim"`. To reinstate the previous functionality, use `optim.fun="nlm"`.

Value

Plug-in bandwidth. If `amise=TRUE` then the minimal scaled PI value is returned too.

References

Chacon, J.E. & Duong, T. (2010) Multivariate plug-in bandwidth selection with unconstrained pilot matrices. *Test*, **19**, 375-398.

Duong, T. & Hazelton, M.L. (2003) Plug-in bandwidth matrices for bivariate kernel density estimation. *Journal of Nonparametric Statistics*, **15**, 17-30.

Sheather, S.J. & Jones, M.C. (1991) A reliable data-based bandwidth selection method for kernel density estimation. *Journal of the Royal Statistical Society Series B*, **53**, 683-690.

Wand, M.P. & Jones, M.C. (1994) Multivariate plug-in bandwidth selection. *Computational Statistics*, **9**, 97-116.

See Also

[Hbcv](#), [Hlscv](#), [Hscv](#)

Examples

```
data(unicef)
Hpi(unicef, pilot="dscalar")
hpi(unicef[,1])
```

hsct

Haematopoietic stem cell transplant

Description

This data set contains the haematopoietic stem cell transplant (HSCT) measurements obtained a flow cytometer from mouse subjects. A flow cytometer measures the spectra of fluorescent signals from biological cell samples to study their properties.

Usage

```
data(hsct)
```

Format

A matrix with 39128 rows and 6 columns. The first column is the FITC-CD45.1 fluorescence (0-1023), the second is the PE-Ly65/Mac1 fluorescence (0-1023), the third is the PI-LiveDead fluorescence (0-1023), the fourth is the APC-CD45.2 fluorescence (0-1023), the fifth is the class label of the cell type (1, 2, 3, 4, 5), the sixth the mouse subject number (5, 6, 9, 12).

Source

Aghaeepour, N., Finak, G., The FlowCAP Consortium, The DREAM Consortium, Hoos, H., Mosmann, T. R., Brinkman, R., Gottardo, R. & Scheuermann, R. H. (2013) Critical assessment of automated flow cytometry data analysis techniques, *Nature Methods* **10**, 228-238.

Hscv

Smoothed cross-validation (SCV) bandwidth selector

Description

SCV bandwidth for 1- to 6-dimensional data.

Usage

```
Hscv(x, nstage=2, pre="sphere", pilot, Hstart, binned,
     bgridsize, amise=FALSE, deriv.order=0, verbose=FALSE, optim.fun="optim")
Hscv.diag(x, nstage=2, pre="scale", pilot, Hstart, binned,
          bgridsize, amise=FALSE, deriv.order=0, verbose=FALSE, optim.fun="optim")
hscv(x, nstage=2, binned=TRUE, bgridsize, plot=FALSE)
```

Arguments

x	vector or matrix of data values
pre	"scale" = <code>pre.scale</code> , "sphere" = <code>pre.sphere</code>
pilot	"amse" = AMSE pilot bandwidths "samse" = single SAMSE pilot bandwidth "unconstr" = single unconstrained pilot bandwidth "dscalar" = single pilot bandwidth for <code>deriv.order>0</code> "dunconstr" = single unconstrained pilot bandwidth for <code>deriv.order>0</code>
Hstart	initial bandwidth matrix, used in numerical optimisation
binned	flag for binned kernel estimation
bgridsize	vector of binning grid sizes
amise	flag to return the minimal scaled SCV value. Default is FALSE.
deriv.order	derivative order
verbose	flag to print out progress information. Default is FALSE.
optim.fun	optimiser function: one of <code>nlm</code> or <code>optim</code>
nstage	number of stages in the SCV bandwidth selector (1 or 2)
plot	flag to display plot of SCV(h) vs h (1-d only). Default is FALSE.

Details

`hscv` is the univariate SCV selector of Jones, Marron & Park (1991). `Hscv` is a multivariate generalisation of this, see Duong & Hazelton (2005). Use `Hscv` for unconstrained bandwidth matrices and `Hscv.diag` for diagonal bandwidth matrices.

The default pilot is "samse" for $d=2$, $r=0$, and "dscalar" otherwise. For SAMSE pilot bandwidths, see Duong & Hazelton (2005). Unconstrained and higher order derivative pilot bandwidths are from Chacon & Duong (2011).

For $d=1$, the selector `hscv` is not always stable for large sample sizes with binning. Examine the plot from `hscv(,plot=TRUE)` to determine the appropriate smoothness of the SCV function. Any non-smoothness is due to the discretised nature of binned estimation.

From `ks` 1.11.1 onwards, the default optimisation function is `optim.fun="optim"`.

For details about the advanced options for `binned`, `Hstart`, see [Hpi](#).

Value

SCV bandwidth. If `amise=TRUE` then the minimal scaled SCV value is returned too.

References

Chacon, J.E. & Duong, T. (2011) Unconstrained pilot selectors for smoothed cross validation. *Australian & New Zealand Journal of Statistics*, **53**, 331-351.

Duong, T. & Hazelton, M.L. (2005) Cross-validation bandwidth matrices for multivariate kernel density estimation. *Scandinavian Journal of Statistics*, **32**, 485-506.

Jones, M.C., Marron, J.S. & Park, B.U. (1991) A simple root n bandwidth selector. *Annals of Statistics*, **19**, 1919-1932.

See Also

[Hbcv](#), [Hlscv](#), [Hpi](#)

Examples

```
data(unicef)
Hscv(unicef)
hscv(unicef[,1])
```

Description

The global errors ISE (Integrated Squared Error), MISE (Mean Integrated Squared Error) and the AMISE (Asymptotic Mean Integrated Squared Error) for 1- to 6-dimensional data. Normal mixture densities have closed form expressions for the MISE and AMISE. So in these cases, we can numerically minimise these criteria to find MISE- and AMISE-optimal matrices.

Usage

```

Hamise.mixt(mus, Sigmas, props, samp, Hstart, deriv.order=0)
Hmise.mixt(mus, Sigmas, props, samp, Hstart, deriv.order=0)
Hamise.mixt.diag(mus, Sigmas, props, samp, Hstart, deriv.order=0)
Hmise.mixt.diag(mus, Sigmas, props, samp, Hstart, deriv.order=0)
hamise.mixt(mus, sigmas, props, samp, hstart, deriv.order=0)
hmise.mixt(mus, sigmas, props, samp, hstart, deriv.order=0)
amise.mixt(H, mus, Sigmas, props, samp, h, sigmas, deriv.order=0)
ise.mixt(x, H, mus, Sigmas, props, h, sigmas, deriv.order=0, binned=FALSE,
        bgridsize)
mise.mixt(H, mus, Sigmas, props, samp, h, sigmas, deriv.order=0)

```

Arguments

mus	(stacked) matrix of mean vectors (>1-d), vector of means (1-d)
Sigmas, sigmas	(stacked) matrix of variance matrices (>1-d), vector of standard deviations (1-d)
props	vector of mixing proportions
samp	sample size
Hstart, hstart	initial bandwidth (matrix), used in numerical optimisation
deriv.order	derivative order
x	matrix of data values
H, h	bandwidth (matrix)
binned	flag for binned kernel estimation. Default is FALSE.
bgridsize	vector of binning grid sizes

Details

ISE is a random variable that depends on the data x . MISE and AMISE are non-random and don't depend on the data. For normal mixture densities, ISE, MISE and AMISE have exact formulas for all dimensions.

Value

Unconstrained MISE- or AMISE-optimal bandwidth matrix. ISE, MISE or AMISE value.

References

Chacon J.E., Duong, T. & Wand, M.P. (2011). Asymptotics for general multivariate kernel density derivative estimators. *Statistica Sinica*, **21**, 807-840.

Examples

```

x <- rmvnorm.mixt(100)
Hamise.mixt(samp=nrow(x), mus=rep(0,2), Sigmas=var(x), props=1, deriv.order=1)

```

kcde *Kernel cumulative distribution/survival function estimate*

Description

Kernel cumulative distribution/survival function estimate for 1- to 3-dimensional data.

Usage

```
kcde(x, H, h, gridsize, gridtype, xmin, xmax, supp=3.7, eval.points,
     binned, bgridsize, positive=FALSE, adj.positive, w, verbose=FALSE,
     tail.flag="lower.tail")
Hpi.kcde(x, nstage=2, pilot, Hstart, binned, bgridsize, amise=FALSE,
         verbose=FALSE, optim.fun="optim")
Hpi.diag.kcde(x, nstage=2, pilot, Hstart, binned, bgridsize, amise=FALSE,
              verbose=FALSE, optim.fun="optim")
hpi.kcde(x, nstage=2, binned, amise=FALSE)

## S3 method for class 'kcde'
predict(object, ..., x)
```

Arguments

x	matrix of data values
H,h	bandwidth matrix/scalar bandwidth. If these are missing, then Hpi.kcde or hpi.kcde is called by default.
gridsize	vector of number of grid points
gridtype	not yet implemented
xmin,xmax	vector of minimum/maximum values for grid
supp	effective support for standard normal
eval.points	vector or matrix of points at which estimate is evaluated
binned	flag for binned estimation. Default is FALSE.
bgridsize	vector of binning grid sizes
positive	flag if 1-d data are positive. Default is FALSE.
adj.positive	adjustment applied to positive 1-d data
w	not yet implemented
verbose	flag to print out progress information. Default is FALSE.
tail.flag	"lower.tail" = cumulative distribution, "upper.tail" = survival function
nstage	number of stages in the plug-in bandwidth selector (1 or 2)
pilot	"dscalar" = single pilot bandwidth (default for Hpi.diag.kcde "dunconstr" = single unconstrained pilot bandwidth (default for Hpi.kcde)
Hstart	initial bandwidth matrix, used in numerical optimisation

amise	flag to return the minimal scaled PI value
optim.fun	optimiser function: one of nlm or optim
object	object of class kcde
...	other parameters

Details

If `tail.flag="lower.tail"` then the cumulative distribution function $\Pr(\mathbf{X} \leq \mathbf{x})$ is estimated, otherwise if `tail.flag="upper.tail"`, it is the survival function $\Pr(\mathbf{X} > \mathbf{x})$. For $d > 1$, $\Pr(\mathbf{X} \leq \mathbf{x}) \neq 1 - \Pr(\mathbf{X} > \mathbf{x})$.

If the bandwidth `H` is missing in `kcde`, then the default bandwidth is the plug-in selector `Hpi.kcde`. Likewise for missing `h`. No pre-scaling/pre-sphering is used since the `Hpi.kcde` is not invariant to translation/dilation.

From `ks` 1.11.1 onwards, the default optimisation function is `optim.fun="optim"`.

The effective support, binning, grid size, grid range, positive parameters are the same as [kde](#).

Value

A kernel cumulative distribution estimate is an object of class `kcde` which is a list with fields:

<code>x</code>	data points - same as input
<code>eval.points</code>	vector or list of points at which the estimate is evaluated
<code>estimate</code>	cumulative distribution/survival function estimate at <code>eval.points</code>
<code>h</code>	scalar bandwidth (1-d only)
<code>H</code>	bandwidth matrix
<code>gridtype</code>	"linear"
<code>gridded</code>	flag for estimation on a grid
<code>binned</code>	flag for binned estimation
<code>names</code>	variable names
<code>w</code>	weights
<code>tail</code>	"lower.tail"=cumulative distribution, "upper.tail"=survival function

References

Duong, T. (2016) Non-parametric smoothed estimation of multivariate cumulative distribution and survival functions, and receiver operating characteristic curves. *Journal of the Korean Statistical Society*, **45**, 33-50.

See Also

[kde](#), [plot.kcde](#)

Examples

```
library(MASS)
data(iris)
Fhat <- kcde(iris[,1:2])
predict(Fhat, x=as.matrix(iris[,1:2]))

## See other examples in ? plot.kcde
```

kcopula

Kernel copula (density) estimate

Description

Kernel copula and copula density estimator for 2-dimensional data.

Usage

```
kcopula(x, H, hs, gridsize, gridtype, xmin, xmax, supp=3.7, eval.points,
        binned, bgridsize, w, verbose=FALSE, marginal="kernel")
kcopula.de(x, H, gridsize, gridtype, xmin, xmax, supp=3.7,
           eval.points, binned, bgridsize, w, verbose=FALSE, compute.cont=TRUE,
           approx.cont=TRUE, marginal="kernel", boundary.supp, boundary.kernel="beta")
```

Arguments

x	matrix of data values
H,hs	bandwidth matrix. If these are missing, Hpi.kcde/Hpi or hpi.kcde/hpi is called by default.
gridsize	vector of number of grid points
gridtype	not yet implemented
xmin,xmax	vector of minimum/maximum values for grid
supp	effective support for standard normal
eval.points	matrix of points at which estimate is evaluated
binned	flag for binned estimation
bgridsize	vector of binning grid sizes
w	vector of weights. Default is a vector of all ones.
verbose	flag to print out progress information. Default is FALSE.
marginal	"kernel" = kernel cdf or "empirical" = empirical cdf to calculate pseudo-uniform values. Default is "kernel".
compute.cont	flag for computing 1% to 99% probability contour levels. Default is TRUE.
approx.cont	flag for computing approximate probability contour levels. Default is TRUE.
boundary.supp	effective support for boundary region
boundary.kernel	"beta" = 2nd form of beta boundary kernel, "linear" = linear boundary kernel

Details

For kernel copula estimates, a transformation approach is used to account for the boundary effects. If H is missing, the default is `Hpi.kcde`; if h_s are missing, the default is `hpi.kcde`.

For kernel copula density estimates, for those points which are in the interior region, the usual kernel density estimator (`kde`) is used. For those points in the boundary region, a product beta kernel based on the boundary corrected univariate beta kernel of Chen (1999) is used (`kde.boundary`). If H is missing, the default is `Hpi.kcde`; if h_s are missing, the default is `hpi`.

The effective support, binning, grid size, grid range parameters are the same as for `kde`.

Value

A kernel copula estimate, output from `kcopula`, is an object of class `kcopula`. A kernel copula density estimate, output from `kcopula.de`, is an object of class `kde`. These two classes of objects have the same fields as `kcde` and `kde` objects respectively, except for

<code>x</code>	pseudo-uniform data points
<code>x.orig</code>	data points - same as input
<code>marginal</code>	marginal function used to compute pseudo-uniform data
<code>boundary</code>	flag for data points in the boundary region (<code>kcopula.de</code> only)

References

Duong, T. (2014) Optimal data-based smoothing for non-parametric estimation of copula functions and their densities. Submitted.

Chen, S.X. (1999). Beta kernel estimator for density functions. *Computational Statistics & Data Analysis*, **31**, 131–145.

See Also

[kcde](#), [kde](#)

Examples

```
library(MASS)
data(fgl)
x <- fgl[,c("RI", "Na")]
Chat <- kcopula(x=x)
plot(Chat, disp="persp", thin=3, col="white", border=1)
```

kda *Kernel discriminant analysis*

Description

Kernel discriminant analysis for 1- to d-dimensional data.

Usage

```
kda(x, x.group, Hs, hs, prior.prob=NULL, gridsize, xmin, xmax, supp=3.7,
    eval.points, binned, bgridsize, w, compute.cont=TRUE, approx.cont=TRUE,
    kde.flag=TRUE)
Hkda(x, x.group, Hstart, bw="plugin", ...)
Hkda.diag(x, x.group, bw="plugin", ...)
hkda(x, x.group, bw="plugin", ...)

## S3 method for class 'kda'
predict(object, ..., x)

compare(x.group, est.group, by.group=FALSE)
compare.kda.cv(x, x.group, bw="plugin", prior.prob=NULL, Hstart, by.group=FALSE,
    verbose=FALSE, recompute=FALSE, ...)
compare.kda.diag.cv(x, x.group, bw="plugin", prior.prob=NULL, by.group=FALSE,
    verbose=FALSE, recompute=FALSE, ...)
```

Arguments

x	matrix of training data values
x.group	vector of group labels for training data
Hs,hs	(stacked) matrix of bandwidth matrices/vector of scalar bandwidths. If these are missing, Hkda or hkda is called by default.
prior.prob	vector of prior probabilities
gridsize	vector of grid sizes
xmin,xmax	vector of minimum/maximum values for grid
supp	effective support for standard normal
eval.points	vector or matrix of points at which estimate is evaluated
binned	flag for binned estimation
bgridsize	vector of binning grid sizes
w	vector of weights. Not yet implemented.
compute.cont	flag for computing 1% to 99% probability contour levels. Default is TRUE.
approx.cont	flag for computing approximate probability contour levels. Default is TRUE.
kde.flag	flag for computing KDE on grid. Default is TRUE.
object	object of class kda

bw	bandwidth: "plugin" = plug-in, "lscv" = LSCV, "scv" = SCV
Hstart	(stacked) matrix of initial bandwidth matrices, used in numerical optimisation
est.group	vector of estimated group labels
by.group	flag to give results also within each group
verbose	flag for printing progress information. Default is FALSE.
recompute	flag for recomputing the bandwidth matrix after excluding the i-th data item
...	other optional parameters for bandwidth selection, see Hpi , Hlscv , Hscv

Details

If the bandwidths `Hs` are missing from `kda`, then the default bandwidths are the plug-in selectors `Hkda(,bw="plugin")`. Likewise for missing `hs`. Valid options for `bw` are "plugin", "lscv" and "scv" which in turn call [Hpi](#), [Hlscv](#) and [Hscv](#).

The effective support, binning, grid size, grid range, positive parameters are the same as [kde](#).

If prior probabilities are known then set `prior.prob` to these. Otherwise `prior.prob=NULL` uses the sample proportions as estimates of the prior probabilities.

As of **ks** 1.8.11, `kda.kde` has been subsumed into `kda`, so all prior calls to `kda.kde` can be replaced by `kda`. To reproduce the previous behaviour of `kda`, the command is `kda(,kde.flag=FALSE)`.

Value

–For `kde.flag=TRUE`, a kernel discriminant analysis is an object of class `kda` which is a list with fields

<code>x</code>	list of data points, one for each group label
<code>estimate</code>	list of density estimates at <code>eval.points</code> , one for each group label
<code>eval.points</code>	vector or list of points that the estimate is evaluated at, one for each group label
<code>h</code>	vector of bandwidths (1-d only)
<code>H</code>	stacked matrix of bandwidth matrices or vector of bandwidths
<code>gridded</code>	flag for estimation on a grid
<code>binned</code>	flag for binned estimation
<code>w</code>	weights
<code>prior.prob</code>	prior probabilities
<code>x.group</code>	group labels - same as input
<code>x.group.estimate</code>	estimated group labels. If the test data <code>eval.points</code> are given then these are classified. Otherwise the training data <code>x</code> are classified.

For `kde.flag=FALSE`, which is always the case for $d > 3$, then only the vector of estimated group labels is returned.

–The result from `Hkda` and `Hkda.diag` is a stacked matrix of bandwidth matrices, one for each training data group. The result from `hkda` is a vector of bandwidths, one for each training group.

–The compare functions create a comparison between the true group labels `x.group` and the estimated ones. It returns a list with fields

cross cross-classification table with the rows indicating the true group and the columns the estimated group

error misclassification rate (MR)

In the case where the test data is independent of the training data, `compare` computes $MR = (\text{number of points wrongly classified})/(\text{total number of points})$. In the case where the test data are not independent e.g. we are classifying the training data set itself, then the cross validated estimate of MR is more appropriate. These are implemented as `compare.kda.cv` (unconstrained bandwidth selectors) and `compare.kda.diag.cv` (for diagonal bandwidth selectors). These functions are only available for $d > 1$.

If by `.group=FALSE` then only the total MR rate is given. If it is set to `TRUE`, then the MR rates for each class are also given (estimated number in group divided by true number).

References

Simonoff, J. S. (1996) *Smoothing Methods in Statistics*. Springer-Verlag. New York

See Also

[plot.kda](#)

Examples

```
set.seed(8192)
x <- c(rnorm.mixt(n=100, mus=1), rnorm.mixt(n=100, mus=-1))
x.gr <- rep(c(1,2), times=c(100,100))
y <- c(rnorm.mixt(n=100, mus=1), rnorm.mixt(n=100, mus=-1))
y.gr <- rep(c(1,2), times=c(100,100))
kda.gr <- kda(x, x.gr)
y.gr.est <- predict(kda.gr, x=y)
compare(y.gr, y.gr.est)

## See other examples in ? plot.kda
```

kdcde

Deconvolution kernel density derivative estimate

Description

Deconvolution kernel density derivative estimate for 1- to 6-dimensional data.

Usage

```
kdcde(x, H, h, Sigma, sigma, reg, bgridsize, gridsize, binned,
      verbose=FALSE, ...)
dckde(...)
```

Arguments

x	matrix of data values
H, h	bandwidth matrix/scalar bandwidth. If these are missing, Hpi or hpi is called by default.
Sigma, sigma	error variance matrix
reg	regularisation parameter
gridsize	vector of number of grid points
binned	flag for binned estimation
bgridsize	vector of binning grid sizes
verbose	flag to print out progress information. Default is FALSE.
...	other parameters to kde

Details

A weighted kernel density estimate is utilised to perform the deconvolution. The weights are obtained from a quadratic programming problem, and then input into `kde(, w=)`. This weighted estimate also requires an estimate of the error variance matrix from repeated observations, and of the regularisation parameter. If the latter is missing, it is calculated internally using a 5-fold cross validation method. See Hazelton & Turlach (2009). `dckde` is an alias for `kdcde`.

If the bandwidth `H` is missing from `kde`, then the default bandwidth is the plug-in selector `Hpi`. Likewise for missing `h`.

The effective support, binning, grid size, grid range, positive parameters are the same as [kde](#).

Value

A deconvolution kernel density derivative estimate is an object of class `kde` which is a list with fields:

x	data points - same as input
eval.points	vector or list of points at which the estimate is evaluated
estimate	density estimate at <code>eval.points</code>
h	scalar bandwidth (1-d only)
H	bandwidth matrix
gridtype	"linear"
gridded	flag for estimation on a grid
binned	flag for binned estimation
names	variable names
w	weights
cont	probability contour levels (if <code>compute.cont=TRUE</code>)

References

Hazelton, M. L. & Turlach, B. A. (2009), Nonparametric density deconvolution by weighted kernel density estimators, *Statistics and Computing*, **19**, 217-228.

See Also[kde](#)**Examples**

```

data(air)
air <- air[, c("date", "time", "co2", "pm10")]
air2 <- reshape(air, idvar="date", timevar="time", direction="wide")
air <- as.matrix(na.omit(air2[,c("co2.20:00", "pm10.20:00")]))
Sigma.air <- diag(c(var(air2[, "co2.19:00"] - air2[, "co2.21:00"], na.rm=TRUE),
  var(air2[, "pm10.19:00"] - air2[, "pm10.21:00"], na.rm=TRUE)))
fhat.air.dec <- kdcde(x=air, Sigma=Sigma.air, reg=0.00021, verbose=TRUE)
plot(fhat.air.dec, drawlabels=FALSE, display="filled.contour", lwd=1)

```

kdde

*Kernel density derivative estimate***Description**

Kernel density derivative estimate for 1- to 6-dimensional data.

Usage

```

kdde(x, H, h, deriv.order=0, gridsize, gridtype, xmin, xmax, supp=3.7,
  eval.points, binned, bgridsize, positive=FALSE, adj.positive, w,
  deriv.vec=TRUE, verbose=FALSE)
kcurv(fhat, compute.cont=TRUE)

```

```

## S3 method for class 'kdde'
predict(object, ..., x)

```

Arguments

x	matrix of data values
H, h	bandwidth matrix/scalar bandwidth. If these are missing, Hpi or hpi is called by default.
deriv.order	derivative order (scalar)
gridsize	vector of number of grid points
gridtype	not yet implemented
xmin, xmax	vector of minimum/maximum values for grid
supp	effective support for standard normal
eval.points	vector or matrix of points at which estimate is evaluated
binned	flag for binned estimation
bgridsize	vector of binning grid sizes

positive	flag if data are positive (1-d, 2-d). Default is FALSE.
adj.positive	adjustment applied to positive 1-d data
w	vector of weights. Default is a vector of all ones.
deriv.vec	flag to compute all derivatives in vectorised derivative. Default is TRUE. If FALSE then only the unique derivatives are computed.
verbose	flag to print out progress information. Default is FALSE.
compute.cont	flag for computing 1% to 99% probability contour levels. Default is TRUE.
fhat	object of class kdde with deriv.order=2
object	object of class kdde
...	other parameters

Details

For each partial derivative, for grid estimation, the estimate is a list whose elements correspond to the partial derivative indices in the rows of `deriv.ind`. For points estimation, the estimate is a matrix whose columns correspond to rows of `deriv.ind`.

If the bandwidth H is missing from `kdde`, then the default bandwidth is the plug-in selector `Hpi`. Likewise for missing `h`.

The effective support, binning, grid size, grid range, positive parameters are the same as [kde](#).

The summary curvature is computed by `kcurv`, i.e.

$$\hat{s}(\mathbf{x}) = -\mathbf{1}\{D^2\hat{f}(\mathbf{x}) < 0\}\text{abs}(|D^2\hat{f}(\mathbf{x})|)$$

where $D^2\hat{f}(\mathbf{x})$ is the kernel Hessian matrix estimate. So \hat{s} calculates the absolute value of the determinant of the Hessian matrix and whose sign is the opposite of the negative definiteness indicator.

Value

A kernel density derivative estimate is an object of class `kdde` which is a list with fields:

x	data points - same as input
eval.points	vector or list of points at which the estimate is evaluated
estimate	density derivative estimate at <code>eval.points</code>
h	scalar bandwidth (1-d only)
H	bandwidth matrix
gridtype	"linear"
gridded	flag for estimation on a grid
binned	flag for binned estimation
names	variable names
w	weights
deriv.order	derivative order (scalar)
deriv.ind	each row is a vector of partial derivative indices

See Also[kde](#)**Examples**

```

set.seed(8192)
x <- rmvnorm.mixt(1000, mus=c(0,0), Sigmas=invvech(c(1,0.8,1)))
fhat <- kdde(x=x, deriv.order=1) ## gradient [df/dx, df/dy]
predict(fhat, x=x[1:5,])

## See other examples in ? plot.kdde

```

kde

*Kernel density estimate***Description**

Kernel density estimate for 1- to 6-dimensional data.

Usage

```

kde(x, H, h, gridsize, gridtype, xmin, xmax, supp=3.7, eval.points,
    binned, bgridsize, positive=FALSE, adj.positive, w,
    compute.cont=TRUE, approx.cont=TRUE, unit.interval=FALSE,
    verbose=FALSE)

## S3 method for class 'kde'
predict(object, ..., x, zero.flag=TRUE)

```

Arguments

x	matrix of data values
H, h	bandwidth matrix/scalar bandwidth. If these are missing, Hpi or hpi is called by default.
gridsize	vector of number of grid points
gridtype	not yet implemented
xmin, xmax	vector of minimum/maximum values for grid
supp	effective support for standard normal
eval.points	vector or matrix of points at which estimate is evaluated
binned	flag for binned estimation.
bgridsize	vector of binning grid sizes
positive	flag if data are positive (1-d, 2-d). Default is FALSE.
adj.positive	adjustment applied to positive 1-d data
w	vector of weights. Default is a vector of all ones.

<code>compute.cont</code>	flag for computing 1% to 99% probability contour levels. Default is TRUE.
<code>approx.cont</code>	flag for computing approximate probability contour levels. Default is TRUE.
<code>unit.interval</code>	flag if 1-d data are bounded on unit interval [0,1]. Default is FALSE.
<code>verbose</code>	flag to print out progress information. Default is FALSE.
<code>object</code>	object of class <code>kde</code>
<code>zero.flag</code>	interpolated values <code>object\$estimate</code> of when <code>x</code> outside of <code>object\$eval.points=0</code> (if TRUE), = nearest <code>object\$estimate</code> (if FALSE)
<code>...</code>	other parameters

Details

For `d=1`, if `h` is missing, the default bandwidth is `hpi`. For `d>1`, if `H` is missing, the default is `Hpi`.

For `d=1`, if `positive=TRUE` then `x` is transformed to $\log(x+\text{adj.positive})$ where the default `adj.positive` is the minimum of `x`. This is known as a log transformation density estimate.

For `d=1, 2, 3`, and if `eval.points` is not specified, then the density estimate is computed over a grid defined by `gridsize` (if `binned=FALSE`) or by `bgridsize` (if `binned=TRUE`). This form is suitable for visualisation in conjunction with the `plot` method.

For `d=4, 5, 6`, and if `eval.points` is not specified, then the density estimate is computed over a grid defined by `gridsize`.

–If `eval.points` is specified, as a vector (`d=1`) or as a matrix (`d=2, 3, 4`), then the density estimate is computed at `eval.points`. This form is suitable for numerical summaries (e.g. maximum likelihood), and is not compatible with the `plot` method. Despite that the density estimate is returned only at `eval.points`, by default, a binned gridded estimate is calculated first and then the density estimate at `eval.points` is computed using the `predict` method. If this default intermediate binned grid estimate is not required, then set `binned=FALSE` to compute directly the exact density estimate at `eval.points`.

Binned kernel estimation is an approximation to the exact kernel estimation and is available for `d=1, 2, 3, 4`. This makes kernel estimators feasible for large samples. The default value of the binning flag `binned` is `n>1` (`d=1`), `n>500` (`d=2`), `n>1000` (`d=3`).

The default `bgridsize, gridsize` are `401` (`d=1`), `rep(151, 2)` (`d=2`), `rep(51, 3)` (`d=3`), `rep(21,4)` (`d=4`).

The effective support for a normal kernel is where all values outside $[-\text{supp}, \text{supp}]^d$ are zero.

The default `xmin` is $\min(x) - H_{\max} * \text{supp}$ and `xmax` is $\max(x) + H_{\max} * \text{supp}$ where `Hmax` is the maximum of the diagonal elements of `H`. The grid produced is the outer product of `c(xmin[1], xmax[1])`, ..., `c(xmin[d], xmax[d])`.

Value

A kernel density estimate is an object of class `kde` which is a list with fields:

<code>x</code>	data points - same as input
<code>eval.points</code>	vector or list of points at which the estimate is evaluated
<code>estimate</code>	density estimate at <code>eval.points</code>
<code>h</code>	scalar bandwidth (1-d only)

H	bandwidth matrix
gridtype	"linear"
gridded	flag for estimation on a grid
binned	flag for binned estimation
names	variable names
w	weights
cont	probability contour levels (if compute.cont=TRUE)

See Also

[plot.kde](#)

Examples

```
## positive data example
data(worldbank)
wb <- as.matrix(na.omit(worldbank[,2:3]))
wb[,2] <- wb[,2]/1000
fhat <- kde(x=wb)
fhat.trans <- kde(x=wb, adj.positive=c(0,0), positive=TRUE)
plot(fhat, xlim=c(0,20), ylim=c(0,80))
plot(fhat.trans, add=TRUE, col=2)
rect(0,0,100,100, lty=2)

## large data example on non-default grid
## 151 x 151 grid = [-5,-4.933,..,5] x [-5,-4.933,..,5]
set.seed(8192)
x <- rmvnorm.mixt(10000, mus=c(0,0), Sigmas=invvech(c(1,0.8,1)))
fhat <- kde(x=x, compute.cont=TRUE, xmin=c(-5,-5), xmax=c(5,5), bgridsize=c(151,151))
plot(fhat)

## See other examples in ? plot.kde
```

kde.boundary

Kernel density estimate for bounded data

Description

Kernel density estimate for bounded 1- to 3-dimensional data.

Usage

```
kde.boundary(x, H, h, gridsize, gridtype, xmin, xmax, supp=3.7, eval.points,
  binned=FALSE, bgridsize, w, compute.cont=TRUE, approx.cont=TRUE,
  boundary.supp, boundary.kernel="beta", verbose=FALSE)
```

Arguments

x	matrix of data values
H,h	bandwidth matrix/scalar bandwidth. If these are missing, Hpi or hpi is called by default.
gridsize	vector of number of grid points
gridtype	not yet implemented
xmin,xmax	vector of minimum/maximum values for grid
supp	effective support for standard normal
eval.points	vector or matrix of points at which estimate is evaluated
binned	flag for binned estimation.
bgridsize	vector of binning grid sizes
w	vector of weights. Default is a vector of all ones.
compute.cont	flag for computing 1% to 99% probability contour levels. Default is TRUE.
approx.cont	flag for computing approximate probability contour levels. Default is TRUE.
boundary.supp	effective support for boundary region
boundary.kernel	"beta" = 2nd form of beta boundary kernel, "linear" = linear boundary kernel
verbose	flag to print out progress information. Default is FALSE.

Details

There are two forms of density estimates which are suitable for bounded data, based on the modifying the kernel function. For `boundary.kernel="beta"`, the 2nd form of the Beta boundary kernel of Chen (1999) is employed. It is suited for rectangular data boundaries.

For `boundary.kernel="linear"`, the linear boundary kernel of Hazelton & Marshall (2009) is employed. It is suited for arbitrarily shaped data boundaries, though it is currently only implemented for rectangular boundaries.

Value

A kernel density estimate for bounded data is an object of class `kde`.

References

Chen, S. X. (1999) Beta kernel estimators for density functions. *Computational Statistics and Data Analysis*, **31**, 131-145.

Hazelton, M. L. & Marshall, J. C. (2009) Linear boundary kernels for bivariate density estimation. *Statistics and Probability Letters*, **79**, 999-1003.

See Also

[kde](#)

Examples

```

data(worldbank)
wb <- as.matrix(na.omit(worldbank[,c("internet", "ag.value")]))
fhat <- kde(x=wb)
fhat.beta <- kde.boundary(x=wb, xmin=c(0,0), xmax=c(100,100), boundary.kernel="beta")
fhat.LB <- kde.boundary(x=wb, xmin=c(0,0), xmax=c(100,100), boundary.kernel="linear")

plot(fhat, xlim=c(0,100), ylim=c(0,100))
plot(fhat.beta, add=TRUE, col=2)
rect(0,0,100,100, lty=2)
plot(fhat, xlim=c(0,100), ylim=c(0,100))
plot(fhat.LB, add=TRUE, col=3)
rect(0,0,100,100, lty=2)

```

kde.local.test

*Kernel density based local two-sample comparison test***Description**

Kernel density based local two-sample comparison test for 1- to 6-dimensional data.

Usage

```

kde.local.test(x1, x2, H1, H2, h1, h2, fhat1, fhat2, gridsize, binned,
  bgridsize, verbose=FALSE, supp=3.7, mean.adj=FALSE, signif.level=0.05,
  min.ESS, xmin, xmax)

```

Arguments

x1,x2	vector/matrix of data values
H1,H2,h1,h2	bandwidth matrices/scalar bandwidths. If these are missing, Hpi or hpi is called by default.
fhat1,fhat2	objects of class kde
binned	flag for binned estimation
gridsize	vector of grid sizes
bgridsize	vector of binning grid sizes
verbose	flag to print out progress information. Default is FALSE.
supp	effective support for normal kernel
mean.adj	flag to compute second order correction for mean value of critical sampling distribution. Default is FALSE. Currently implemented for $d \leq 2$ only.
signif.level	significance level. Default is 0.05.
min.ESS	minimum effective sample size. See below for details.
xmin,xmax	vector of minimum/maximum values for grid

Details

The null hypothesis is $H_0(\mathbf{x}) : f_1(\mathbf{x}) = f_2(\mathbf{x})$ where f_1, f_2 are the respective density functions. The measure of discrepancy is $U(\mathbf{x}) = [f_1(\mathbf{x}) - f_2(\mathbf{x})]^2$. Duong (2013) shows that the test statistic obtained, by substituting the KDEs for the true densities, has a null distribution which is asymptotically chi-squared with 1 d.f.

The required input is either x_1, x_2 and H_1, H_2 , or $\text{fhat1}, \text{fhat2}$, i.e. the data values and bandwidths or objects of class `kde`. In the former case, the `kde` objects are created. If the H_1, H_2 are missing then the default are the plugin selectors `Hpi`. Likewise for missing h_1, h_2 .

The `mean.adj` flag determines whether the second order correction to the mean value of the test statistic should be computed. `min.ESS` is borrowed from Godtliebsen et al. (2002) to reduce spurious significant results in the tails, though by it is usually not required for small to moderate sample sizes.

Value

A kernel two-sample local significance is an object of class `kde.loctest` which is a list with fields:

<code>fhat1, fhat2</code>	kernel density estimates, objects of class <code>kde</code>
<code>chisq</code>	chi squared test statistic
<code>pvalue</code>	matrix of local p-values at each grid point
<code>fhat.diff</code>	difference of KDEs
<code>mean.fhat.diff</code>	mean of the test statistic
<code>var.fhat.diff</code>	variance of the test statistic
<code>fhat.diff.pos</code>	binary matrix to indicate locally significant $\text{fhat1} > \text{fhat2}$
<code>fhat.diff.neg</code>	binary matrix to indicate locally significant $\text{fhat1} < \text{fhat2}$
<code>n1, n2</code>	sample sizes
<code>H1, H2, h1, h2</code>	bandwidth matrices/scalar bandwidths

References

Duong, T. (2013) Local significant differences from non-parametric two-sample tests. *Journal of Nonparametric Statistics*, **25**, 635-645.

Godtliebsen, F., Marron, J.S. & Chaudhuri, P. (2002) Significance in scale space for bivariate density estimation. *Journal of Computational and Graphical Statistics*, **11**, 1-22.

See Also

[kde.test](#), [plot.kde.loctest](#)

Examples

```
library(MASS)
x1 <- crabs[crabs$sp=="B", 4]
x2 <- crabs[crabs$sp=="O", 4]
loct <- kde.local.test(x1=x1, x2=x2)
plot(loct)
```

```
## see examples in ? plot.kde.loctest
```

kde.test

Kernel density based global two-sample comparison test

Description

Kernel density based global two-sample comparison test for 1- to 6-dimensional data.

Usage

```
kde.test(x1, x2, H1, H2, h1, h2, psi1, psi2, var.fhat1, var.fhat2,
         binned=FALSE, bgridsize, verbose=FALSE)
```

Arguments

x1,x2	vector/matrix of data values
H1,H2,h1,h2	bandwidth matrices/scalar bandwidths. If these are missing, <code>Hpi.kfe</code> , <code>hpi.kfe</code> is called by default.
psi1,psi2	zero-th order kernel functional estimates
var.fhat1,var.fhat2	sample variance of KDE estimates evaluated at x1, x2
binned	flag for binned estimation. Default is FALSE.
bgridsize	vector of binning grid sizes
verbose	flag to print out progress information. Default is FALSE.

Details

The null hypothesis is $H_0 : f_1 \equiv f_2$ where f_1, f_2 are the respective density functions. The measure of discrepancy is the integrated squared error (ISE) $T = \int [f_1(\mathbf{x}) - f_2(\mathbf{x})]^2 d\mathbf{x}$. If we rewrite this as $T = \psi_{0,1} - \psi_{0,12} - \psi_{0,21} + \psi_{0,2}$ where $\psi_{0,uv} = \int f_u(\mathbf{x})f_v(\mathbf{x}) d\mathbf{x}$, then we can use kernel functional estimators. This test statistic has a null distribution which is asymptotically normal, so no bootstrap resampling is required to compute an approximate p-value.

If H1,H2 are missing then the plug-in selector `Hpi.kfe` is automatically called by `kde.test` to estimate the functionals with `kfe(,deriv.order=0)`. Likewise for missing h1,h2.

As of **ks** 1.8.8, `kde.test(,binned=TRUE)` invokes binned estimation for the computation of the bandwidth selectors, and not the test statistic and p-value.

Value

A kernel two-sample global significance test is a list with fields:

Tstat	T statistic
zstat	z statistic - normalised version of Tstat
pvalue	p-value of the double sided test
mean, var	mean and variance of null distribution
var.fhat1, var.fhat2	sample variances of KDE values evaluated at data points
n1, n2	sample sizes
H1, H2	bandwidth matrices
psi1, psi12, psi21, psi2	kernel functional estimates

References

Duong, T., Goud, B. & Schauer, K. (2012) Closed-form density-based framework for automatic detection of cellular morphology changes. *PNAS*, **109**, 8382-8387.

See Also

[kde.local.test](#)

Examples

```
set.seed(8192)
samp <- 1000
x <- rnorm.mixt(n=samp, mus=0, sigmas=1, props=1)
y <- rnorm.mixt(n=samp, mus=0, sigmas=1, props=1)
kde.test(x1=x, x2=y)$pvalue ## accept H0: f1=f2

library(MASS)
data(crabs)
x1 <- crabs[crabs$sp=="B", c(4,6)]
x2 <- crabs[crabs$sp=="O", c(4,6)]
kde.test(x1=x1, x2=x2)$pvalue ## reject H0: f1=f2
```

kde.truncate

Truncated kernel density derivative estimate

Description

Truncated kernel density derivative estimate for 2-dimensional data.

Usage

```
kde.truncate(fhat, boundary)
kdde.truncate(fhat, boundary)
```

Arguments

fhat	object of class kde or kdde
boundary	two column matrix delimiting the boundary for truncation
...	other parameters

Details

A simple truncation is performed on the kernel estimator. All the points in the estimation grid which are outside of the regions delimited by boundary are set to 0, and their probability mass is distributed proportionally to the density (derivative) value.

Value

A truncated kernel density (derivative) estimate inherits the same object class as the input estimate.

See Also

[kde](#), [kdde](#)

Examples

```
library(oz)
data(grevillea)
wa.coast <- ozRegion(section=1)
wa.polygon <- cbind(wa.coast$lines[[1]]$x, wa.coast$lines[[1]]$y)
fhat <- kde(x=grevillea)
fhat <- kde.truncate(fhat, wa.polygon)
oz(section=1, xlim=c(114.75, 121.5), ylim=c(-33, -31.5))
plot(fhat, add=TRUE, cont=seq(10,90,by=10), col=2, drawlabels=FALSE, drawpoints=TRUE)
```

kdr

Kernel density ridge estimation

Description

Kernel density ridge estimation for 2- to 3-dimensional data.

Usage

```
kdr(x, y, H, p=1, max.iter=400, tol.iter, tol.seg, min.seg.size,
    keep.path=FALSE, gridsize, xmin, xmax, binned, bgridsize, w, fhat,
    density.cutoff, verbose=FALSE)
```


Arguments

x	matrix of data values
y	matrix of initial values
p	dimension of density ridge
H	bandwidth matrix/scalar bandwidth. If missing, <code>Hpi(x, deriv, order=2)</code> is called by default.
max.iter	maximum number of iterations. Default is 400.
tol.iter	distance under which two successive iterations are considered convergent. Default is $0.001 * \text{min marginal IQR of } x$.
tol.seg	distance under which two segments are considered to form one segment. Default is $0.01 * \text{max marginal IQR of } x$.
min.seg.size	minimum length of a segment of a density ridge. Default is <code>round(0.001*nrow(y), 0)</code> .
keep.path	flag to store the density gradient ascent paths. Default is FALSE.
gridsize	vector of number of grid points
xmin, xmax	vector of minimum/maximum values for grid
binned	flag for binned estimation.
bgridsize	vector of binning grid sizes
w	vector of weights. Default is a vector of all ones.
fhat	kde of x. If missing <code>kde(x=x, w=w)</code> is executed.
density.cutoff	density threshold under which the y are excluded from the density ridge estimation. Default is <code>contourLevels(fhat, cont=99)</code> .
verbose	flag to print out progress information. Default is FALSE.
...	other parameters to kde

Details

Kernel density ridge estimation is based on reduced dimension kernel mean shift. *** To do. ***
See Ozertem & Erdogmus (2011).

If y is missing, then it defaults to the grid of size `gridsize` spanning from `xmin` to `xmax`.

If the bandwidth H is missing, then the default bandwidth is the plug-in selector for the density gradient `Hpi(x, deriv, order=2)`. Any bandwidth that is suitable for the density Hessian is also suitable for the kernel density ridge.

Value

A kernel density ridge set is an object of class `kdr` which is a list with fields:

x, y	data points - same as input
end.points	matrix of final iterates starting from y
H	bandwidth matrix
names	variable names

<code>tol.iter</code> , <code>tol.clust</code> , <code>min.seg.size</code>	tuning parameter values - same as input
<code>binned</code>	flag for binned estimation
<code>names</code>	variable names
<code>w</code>	weights
<code>path</code>	list of density gradient ascent paths where <code>path[[i]]</code> is the path of <code>y[i,]</code> (only if <code>keep.path=TRUE</code>)

References

Ozertem, U. & Erdogmus, D. (2011), Locally defined principal curves and surfaces, *Journal of Machine Learning Research*, **12**, 1249-1286.

See Also

[kde](#)

Examples

```
library(maps)
data(quake)
quake <- quake[quake$prof==1,] ## Pacific Ring of Fire
quake$long[quake$long<0] <- quake$long[quake$long<0] + 360
quake <- quake[, c("long", "lat")]
data(plate) ## tectonic plate boundaries
plate <- plate[plate$long < -20 | plate$long > 20,]
plate$long[plate$long<0 & !is.na(plate$long)] <- plate$long[plate$long<0
& !is.na(plate$long)] + 360

dr.quake <- kdr(x=quake, xmin=c(70,-70), xmax=c(310, 80))
map("world2", xlim=c(85, 305), ylim=c(-70, 70), mar=c(0,0,0,0), interior=FALSE, lty=2)
lines(plate[,1:2], col=3, lwd=2)
points(dr.quake$end.points, cex=0.5, pch=16, col=2)
```

kfe

Kernel functional estimate

Description

Kernel functional estimate for 1- to 6-dimensional data.

Usage

```

kfe(x, G, deriv.order, inc=1, binned, bin.par, bgridsize, deriv.vec=TRUE,
    add.index=TRUE, verbose=FALSE)
Hpi.kfe(x, nstage=2, pilot, pre="sphere", Hstart, binned=FALSE,
    bgridsize, amise=FALSE, deriv.order=0, verbose=FALSE, optim.fun="optim")
Hpi.diag.kfe(x, nstage=2, pilot, pre="scale", Hstart, binned=FALSE,
    bgridsize, amise=FALSE, deriv.order=0, verbose=FALSE, optim.fun="optim")
hpi.kfe(x, nstage=2, binned=FALSE, bgridsize, amise=FALSE, deriv.order=0)

```

Arguments

x	vector/matrix of data values
nstage	number of stages in the plug-in bandwidth selector (1 or 2)
pilot	"dscalar" = single pilot bandwidth (default) "dunconstr" = single unconstrained pilot bandwidth
pre	"scale" = pre.scale , "sphere" = pre.sphere
Hstart	initial bandwidth matrix, used in numerical optimisation
binned	flag for binned estimation
bgridsize	vector of binning grid sizes
amise	flag to return the minimal scaled PI value
deriv.order	derivative order
verbose	flag to print out progress information. Default is FALSE.
optim.fun	optimiser function: one of nlm or optim
G	pilot bandwidth matrix
inc	0=exclude diagonal, 1=include diagonal terms in kfe calculation
bin.par	binning parameters - output from binning
deriv.vec	flag to compute duplicated partial derivatives in the vectorised form. Default is FALSE.
add.index	flag to output derivative indices matrix. Default is true.

Details

Hpi.kfe is the optimal plug-in bandwidth for r -th order kernel functional estimator based on the unconstrained pilot selectors of Chacon & Duong (2010). hpi.kfe is the 1-d equivalent, using the formulas from Wand & Jones (1995, p.70).

kfe does not usually need to be called explicitly by the user.

Value

Plug-in bandwidth matrix for r -th order kernel functional estimator.

References

Chacon, J.E. & Duong, T. (2010) Multivariate plug-in bandwidth selection with unconstrained pilot matrices. *Test*, **19**, 375-398.

Wand, M.P. & Jones, M.C. (1995) *Kernel Smoothing*. Chapman & Hall/CRC, London.

See Also

[kde.test](#)

kfs

Kernel feature significance

Description

Kernel feature significance for 1- to 6-dimensional data.

Usage

```
kfs(x, H, h, deriv.order=2, gridsize, gridtype, xmin, xmax, supp=3.7,
    eval.points, binned, bgridsize, positive=FALSE, adj.positive, w,
    verbose=FALSE, signif.level=0.05)
```

Arguments

x	matrix of data values
H, h	bandwidth matrix/scalar bandwidth. If these are missing, Hpi or hpi is called by default.
deriv.order	derivative order (scalar)
gridsize	vector of number of grid points
gridtype	not yet implemented
xmin, xmax	vector of minimum/maximum values for grid
supp	effective support for standard normal
eval.points	vector or matrix of points at which estimate is evaluated
binned	flag for binned estimation
bgridsize	vector of binning grid sizes
positive	flag if 1-d data are positive. Default is FALSE.
adj.positive	adjustment applied to positive 1-d data
w	vector of weights. Default is a vector of all ones.
verbose	flag to print out progress information. Default is FALSE.
signif.level	overall level of significance for hypothesis tests. Default is 0.05.

Details

Feature significance is based on significance testing of the gradient (first derivative) and curvature (second derivative) of a kernel density estimate. Only the latter is currently implemented, and is also known as significant modal regions.

The hypothesis test at a grid point \boldsymbol{x} is $H_0(\boldsymbol{x}) : Hf(\boldsymbol{x}) < 0$, i.e. the density Hessian matrix $Hf(\boldsymbol{x})$ is negative definite. The p -values are computed for each \boldsymbol{x} using that the test statistic is approximately chi-squared distributed with $d(d + 1)/2$ d.f. We then use a Hochberg-type simultaneous testing procedure, based on the ordered p -values, to control the overall level of significance to be signif.level. If $H_0(\boldsymbol{x})$ is rejected then \boldsymbol{x} belongs to a significant modal region.

The computations are based on `kdde(x, deriv.order=2)` so `kfs` inherits its behaviour from `kdde`. If the bandwidth `H` is missing from `kfs`, then the default bandwidth is the plug-in selector `Hpi(, deriv.order=2)`. Likewise for missing `h`. The effective support, binning, grid size, grid range, positive parameters are the same as `kde`.

This function is similar to the `featureSignif` function in the **feature** package, except that it accepts unconstrained bandwidth matrices.

Value

A kernel feature significance estimate is an object of class `kfs` which is a list with fields

<code>x</code>	data points - same as input
<code>eval.points</code>	vector or list of points at which the estimate is evaluated
<code>estimate</code>	binary matrix for significant feature at <code>eval.points</code> : 0 = not signif., 1 = signif.
<code>h</code>	scalar bandwidth (1-d only)
<code>H</code>	bandwidth matrix
<code>gridtype</code>	"linear"
<code>gridded</code>	flag for estimation on a grid
<code>binned</code>	flag for binned estimation
<code>names</code>	variable names
<code>w</code>	weights
<code>deriv.order</code>	derivative order (scalar)
<code>deriv.ind</code>	each row is a vector of partial derivative indices.

This is the same structure as a `kdde` object, except that `estimate` is a binary matrix rather than real-valued.

References

- Chaudhuri, P. & Marron, J.S. (1999) SiZer for exploration of structures in curves. *Journal of the American Statistical Association*, **94**, 807-823.
- Duong, T., Cowling, A., Koch, I. & Wand, M.P. (2008) Feature significance for multivariate kernel density estimation. *Computational Statistics and Data Analysis*, **52**, 4225-4242.
- Godtliebsen, F., Marron, J.S. & Chaudhuri, P. (2002) Significance in scale space for bivariate density estimation. *Journal of Computational and Graphical Statistics*, **11**, 1-22.

See Also

[kdde](#), [plot.kfs](#)

Examples

```
## see example is ? plot.kfs
```

kms	<i>Kernel mean shift clustering</i>
-----	-------------------------------------

Description

Kernel mean shift clustering for 2- to 6-dimensional data.

Usage

```
kms(x, y, H, max.iter=400, tol.iter, tol.clust, min.clust.size, merge=TRUE,
    keep.path=FALSE, verbose=FALSE)
```

```
## S3 method for class 'kms'
summary(object, ...)
```

Arguments

x	matrix of data values
y	matrix of candidate data values for which the mean shift will estimate their cluster labels. If missing, $y=x$.
H	bandwidth matrix/scalar bandwidth. If missing, <code>Hpi(x, deriv, order=1)</code> is called by default.
max.iter	maximum number of iterations. Default is 400.
tol.iter	distance under which two successive iterations are considered convergent. Default is $0.001 \cdot \min$ marginal IQR of x .
tol.clust	distance under which two cluster modes are considered to form one cluster. Default is $0.01 \cdot \max$ marginal IQR of x .
min.clust.size	minimum cluster size (cardinality). Default is $0.01 \cdot \text{nrow}(y)$.
merge	flag to merge clusters which are smaller than <code>min.clust.size</code> . Default is TRUE.
keep.path	flag to store the density gradient ascent paths. Default is FALSE.
verbose	flag to print out progress information. Default is FALSE.
object	object of class <code>kms</code>
...	other parameters

Details

Mean shift clustering belongs to the class of modal or density-based clustering methods. The mean shift recurrence of the candidate point \mathbf{x} is $\mathbf{x}_{j+1} = \mathbf{x}_j + \mathbf{H}D\hat{f}(\mathbf{x}_j)/\hat{f}(\mathbf{x}_j)$ where $j \geq 0$ and $\mathbf{x}_0 = \mathbf{x}$. The sequence $\{\mathbf{x}_0, \mathbf{x}_1, \dots\}$ follows the density gradient ascent paths to converge to a local mode of the density estimate \hat{f} . Hence \mathbf{x} is iterated until it converges to its local mode, and this determines its cluster label.

The mean shift recurrence is terminated if successive iterations are less than `tol.iter` or the maximum number of iterations `max.iter` is reached. Final iterates which are less than `tol.clust` distance apart are considered to form a single cluster. If `merge=TRUE` then the clusters whose cardinality is less than `min.clust.size` are iteratively merged with their nearest cluster.

If the bandwidth `H` is missing, then the default bandwidth is the plug-in selector for the density gradient `Hpi(x,deriv.order=1)`. Any bandwidth that is suitable for the density gradient is also suitable for the mean shift.

Value

A kernel mean shift clusters set is an object of class `kms` which is a list with fields:

<code>x,y</code>	data points - same as input
<code>end.points</code>	matrix of final iterates starting from <code>y</code>
<code>H</code>	bandwidth matrix
<code>label</code>	vector of cluster labels
<code>nclust</code>	number of clusters
<code>nclust.table</code>	frequency table of cluster labels
<code>mode</code>	matrix of cluster modes
<code>names</code>	variable names
<code>tol.iter,tol.clust,min.clust.size</code>	tuning parameter values - same as input
<code>path</code>	list of density gradient ascent paths where <code>path[[i]]</code> is the path of <code>y[i,]</code> (only if <code>keep.path=TRUE</code>)

References

Chacon, J.E. & Duong, T. (2013) Data-driven density estimation, with applications to nonparametric clustering and bump hunting. *Electronic Journal of Statistics*, **7**, 499-532.

Comaniciu, D. & Meer, P. (2002). Mean shift: a robust approach toward feature space analysis. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, **24**, 603-619.

See Also

[kde](#)

Examples

```
library(MASS)
data(crabs)
kms.crabs <- kms(x=crabs[,c("FL", "CW")])
plot(kms.crabs$x, col=kms.crabs$label)
summary(kms.crabs)
```

kroc

*Kernel receiver operating characteristic (ROC) curve***Description**

Kernel receiver operating characteristic (ROC) curve for 1- to 3-dimensional data.

Usage

```
kroc(x1, x2, H1, h1, hy, gridsize, gridtype, xmin, xmax, supp=3.7, eval.points,
     binned, bgridsize, positive=FALSE, adj.positive, w, verbose=FALSE)
```

```
## S3 method for class 'kroc'
predict(object, ..., x)
## S3 method for class 'kroc'
summary(object, ...)
```

Arguments

<code>x, x1, x2</code>	vector/matrix of data values
<code>H1, h1, hy</code>	bandwidth matrix/scalar bandwidths. If these are missing, <code>hpi.kcde</code> , <code>hpi.kcde</code> is called by default.
<code>gridsize</code>	vector of number of grid points
<code>gridtype</code>	not yet implemented
<code>xmin, xmax</code>	vector of minimum/maximum values for grid
<code>supp</code>	effective support for standard normal
<code>eval.points</code>	not yet implemented
<code>binned</code>	flag for binned estimation
<code>bgridsize</code>	vector of binning grid sizes
<code>positive</code>	flag if 1-d data are positive. Default is FALSE.
<code>adj.positive</code>	adjustment applied to positive 1-d data
<code>w</code>	vector of weights. Default is a vector of all ones.
<code>verbose</code>	flag to print out progress information. Default is FALSE.
<code>object</code>	object of class <code>kroc</code> , output from <code>kroc</code>
<code>...</code>	other parameters

Details

In this set-up, the values in the first sample x_1 should be larger in general than those in the second sample x_2 . The usual method for computing 1-d ROC curves is not valid for multivariate data. Duong (2014), based on Lloyd (1998), develops an alternative formulation $(F_{Y_1}(z), F_{Y_2}(z))$ based on the cumulative distribution functions of $Y_j = \bar{F}_1(\mathbf{X}_j), j = 1, 2$.

If the bandwidth H_1 is missing from `kroc`, then the default bandwidth is the plug-in selector `Hpi.kcde`. Likewise for missing h_1, h_y . A bandwidth matrix H_1 is required for x_1 for $d > 1$, but the second bandwidth h_y is always a scalar since Y_j are 1-d variables.

The effective support, binning, grid size, grid range, positive parameters are the same as [kde](#).

–The summary method for `kroc` objects prints out the summary indices of the ROC curve, as contained in the `indices` field, namely the AUC (area under the curve) and Youden index.

Value

A kernel ROC curve is an object of class `kroc` which is a list with fields:

<code>x</code>	list of data values x_1, x_2 - same as input
<code>eval.points</code>	vector or list of points at which the estimate is evaluated
<code>estimate</code>	ROC curve estimate at <code>eval.points</code>
<code>gridtype</code>	"linear"
<code>gridded</code>	flag for estimation on a grid
<code>binned</code>	flag for binned estimation
<code>names</code>	variable names
<code>w</code>	weights
<code>tail</code>	"lower.tail"
<code>h1</code>	scalar bandwidth for first sample (1-d only)
<code>H1</code>	bandwidth matrix for first sample
<code>hy</code>	scalar bandwidth for ROC curve
<code>indices</code>	summary indices of ROC curve.

References

Duong, T. (2016) Non-parametric smoothed estimation of multivariate cumulative distribution and survival functions, and receiver operating characteristic curves. *Journal of the Korean Statistical Society*, **45**, 33-50.

Lloyd, C. (1998) Using smoothed receiver operating curves to summarize and compare diagnostic systems. *Journal of the American Statistical Association*, **93**, 1356-1364.

See Also

[kcde](#)

Examples

```
samp <- 1000
x <- rnorm.mixt(n=samp, mus=0, sigmas=1, props=1)
y <- rnorm.mixt(n=samp, mus=0.5, sigmas=1, props=1)
Rhat <- kroc(x1=x, x2=y)
summary(Rhat)
predict(Rhat, x=0.5)
```

ksupp	<i>Kernel support estimate</i>
-------	--------------------------------

Description

Kernel support estimate for 2-dimensional data.

Usage

```
ksupp(fhat, cont=95, abs.cont, convex.hull=FALSE)
```

Arguments

fhat	object of class kde
cont	percentage for contour level curve. Default is 95.
abs.cont	absolute density estimate height for contour level curve
convex.hull	flag to compute convex hull of contour level curve. Default is FALSE.

Details

The kernel support estimate is the level set of the density estimate that exceeds the cont percent contour level. If this level set is a simply connected region, then this can suffice to be a conservative estimate of the density support. Otherwise, the convex hull of the level set is advised.

Value

A kernel support estimate is a 2-column matrix which delimits the (convex hull of the) level set of the density estimate fhat.

See Also

[kde](#)

Examples

```

library(oz)
data(grevillea)
fhat <- kde(x=grevillea)
fhat.supp <- ksupp(fhat, convex.hull=TRUE)
plot(fhat, display="filled.contour", cont=seq(10,90,by=10), drawlabels=FALSE)
plot(fhat, cont=95, add=TRUE)
polygon(fhat.supp, lty=2)

```

mixt

Normal and t-mixture distributions

Description

Random generation and density values from normal and t-mixture distributions.

Usage

```

dnorm.mixt(x, mus=0, sigmas=1, props=1)
rnorm.mixt(n=100, mus=0, sigmas=1, props=1, mixt.label=FALSE)
dmvnorm.mixt(x, mus, Sigmas, props=1, verbose=FALSE)
rmvnorm.mixt(n=100, mus=c(0,0), Sigmas=diag(2), props=1, mixt.label=FALSE)
rmvt.mixt(n=100, mus=c(0,0), Sigmas=diag(2), dfs=7, props=1)
dmvt.mixt(x, mus, Sigmas, dfs, props)
mvnorm.mixt.mode(mus, Sigmas, props=1, verbose=FALSE)

```

Arguments

n	number of random variates
x	matrix of quantiles
mus	(stacked) matrix of mean vectors (>1-d) or vector of means (1-d)
Sigmas	(stacked) matrix of variance matrices (>1-d)
sigmas	vector of standard deviations (1-d)
props	vector of mixing proportions
mixt.label	flag to output numeric label indicating mixture component. Default is FALSE.
verbose	flag to print out progress information. Default is FALSE.
dfs	vector of degrees of freedom

Details

`rmvnorm.mixt` and `dmvnorm.mixt` are based on the `rmvnorm` and `dmvnorm` functions from the **mvtnorm** package. Likewise for `rmvt.mixt` and `dmvt.mixt`.

For the normal mixture densities, `mvnorm.mixt.mode` computes the local modes: these are usually very close but not exactly equal to the component means.

Value

Normal and t-mixture random vectors and density values.

Examples

```
## univariate normal mixture
x <- rnorm.mixt(1000, mus=c(-1,1), sigmas=c(0.5, 0.5), props=c(1/2, 1/2))

## bivariate mixtures
mus <- rbind(c(-1,0), c(1, 2/sqrt(3)), c(1,-2/sqrt(3)))
Sigmas <- 1/25*rbind(invvech(c(9, 63/10, 49/4)), invvech(c(9,0,49/4)), invvech(c(9,0,49/4)))
props <- c(3,3,1)/7
dfs <- c(7,3,2)
x <- rmvnorm.mixt(1000, mus=mus, Sigmas=Sigmas, props=props)
y <- rmvt.mixt(1000, mus=mus, Sigmas=Sigmas, dfs=dfs, props=props)

mvnorm.mixt.mode(mus=mus, Sigmas=Sigmas, props=props)
```

plot.histde

Plot for histogram density estimate

Description

Plot for histogram density estimate for 1- and 2-dimensional data.

Usage

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

Arguments

x an object of class histde (output from [histde](#))

... other graphics parameters:

- col plotting colour for density estimate
- col.fun plotting colour function for levels
- col.pt plotting colour for data points
- jitter flag to jitter rug plot (1-d). Default is TRUE.
- xlim,ylim axes limits
- xlab,ylab axes labels
- add flag to add to current plot. Default is FALSE.
- drawpoints flag to draw data points on density estimate. Default is FALSE.
- breaks vector of break values of density estimate. Default is an nbreaks equi-linear sequence over the data range.
- nbreaks number of breaks in breaks sequence
- lty.rect,lwd.rect line type/width for histogram box lines (2-d)

border colour of histogram box lines (2-d)
col.rect colour of histogram bars (1-d)
add.grid flag to add histogram grid (2-d). Default is TRUE.

Details

For histde objects, the function headers for the different dimensional data are

```
## univariate
plot(fhat, xlab, ylab="Density function", add=FALSE, drawpoints=FALSE,
     col.pt="blue", jitter=FALSE, border=1, ...)

## bivariate
plot(fhat, breaks, nbreaks=11, xlab, ylab, zlab="Density function", cex=1,
     pch=1, add=FALSE, drawpoints=FALSE, col, col.fun, col.pt="blue",
     lty.rect=2, cex.text=1, border, lwd.rect=1, col.rect="transparent",
     add.grid=TRUE, ...)
```

The 1-d plot is a standard plot of a histogram generated by `hist`. If `drawpoints=TRUE` then a rug plot is added.

The 2-d plot is similar to the `display="filled.contour"` option from `plot.kde` with the default `nbreaks=11` contour levels. Default colours are the default from the `image` command.

Value

Plots for 1-d and 2-d are sent to graphics window.

See Also

[plot.kde](#)

Examples

```
library(MASS)
data(iris)

## univariate example
fhat <- histde(x=iris[,2])
plot(fhat, border=3, xlab="Sepal length")

## bivariate example
fhat <- histde(x=iris[,2:3])
plot(fhat, drawpoints=TRUE)
box()
```

plot.kcde	<i>Plot for kernel cumulative distribution estimate</i>
-----------	---

Description

Plot for kernel cumulative distribution estimate 1- to 3-dimensional data.

Usage

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

Arguments

x an object of class kcde (output from [kcde](#))
... other graphics parameters used in [plot.kde](#)

Details

For kcde objects, the function headers for the different dimensional data are

```
## univariate  
plot(Fhat, xlab, ylab="Distribution function", add=FALSE, drawpoints=FALSE,  
      col.pt="blue", jitter=FALSE, ...)  
  
## bivariate  
plot(Fhat, display="persp", cont=seq(10,90, by=10), abs.cont, xlab, ylab,  
      zlab="Distribution function", cex=1, pch=1, add=FALSE, drawpoints=FALSE,  
      drawlabels=TRUE, theta=-30, phi=40, d=4, col.pt="blue", col, col.fun,  
      lwd=1, border=NA, thin=1, ...)
```

Value

Plots for 1-d and 2-d are sent to graphics window. Plot for 3-d is sent to RGL window (not yet implemented).

See Also

[plot.kde](#)

Examples

```
library(MASS)  
data(iris)  
Fhat <- kcde(x=iris[,1])  
plot(Fhat, xlab="Sepal.Length")  
Fhat <- kcde(x=iris[,1:2])  
plot(Fhat, thin=3)
```

plot.kda

Plot for kernel discriminant analysis

Description

Plot for kernel discriminant analysis for 1- to 3-dimensional data.

Usage

```
## S3 method for class 'kda'
plot(x, y, y.group, ...)
```

Arguments

x	object of class kda (output from kda)
y	matrix of test data points
y.group	vector of group labels for test data points
...	other graphics parameters: rugsize height of rug-like plot for partition classes (1-d) prior.prob vector of prior probabilities col.part vector of colours for partition classes (1-d, 2-d) and those used in plot.kde

Details

For kda objects, the function headers for the different dimensional data are

```
## univariate
plot(x, y, y.group, prior.prob=NULL, xlim, ylim, xlab="x",
     ylab="Weighted density function", drawpoints=FALSE, col, col.part,
     col.pt, lty, jitter=TRUE, rugsize, ...)

## bivariate
plot(x, y, y.group, prior.prob=NULL, cont=c(25,50,75), abs.cont,
     approx.cont=FALSE, xlim, ylim, xlab, ylab, drawpoints=FALSE,
     drawlabels=TRUE, col, col.part, col.pt, ...)

## trivariate
plot(x, y, y.group, prior.prob=NULL, cont=c(25,50,75), abs.cont,
     approx.cont=FALSE, colors, alphavec, xlab, ylab, zlab,
     drawpoints=FALSE, size=3, col.pt="blue", ...)
```

Value

Plots for 1-d and 2-d are sent to graphics window. Plot for 3-d is sent to RGL window.

See Also

[kda](#), [kde](#)

Examples

```
library(MASS)
data(iris)

## univariate example
ir <- iris[,1]
ir.gr <- iris[,5]
kda.fhat <- kda(x=ir, x.group=ir.gr, xmin=3, xmax=9)
plot(kda.fhat, xlab="Sepal length")

## bivariate example
ir <- iris[,1:2]
ir.gr <- iris[,5]
kda.fhat <- kda(x=ir, x.group=ir.gr)
plot(kda.fhat)

## trivariate example
ir <- iris[,1:3]
ir.gr <- iris[,5]
kda.fhat <- kda(x=ir, x.group=ir.gr)
plot(kda.fhat, drawpoints=TRUE, col.pt=c(2,3,4))
  ## colour=species, transparency=density heights
```

plot.kdde

Plot for kernel density derivative estimate

Description

Plot for kernel density derivative estimate for 1- to 3-dimensional data.

Usage

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

Arguments

x an object of class `kdde` (output from [kdde](#))
 ... other graphics parameters:
 which.deriv.ind index of the partial derivative to be plotted (>1-d)
 and those used in [plot.kde](#)

Details

For kdde objects, the function headers for the different dimensional data are

```
## univariate
plot(fhat, ylab="Density derivative function", ...)

## bivariate
plot(fhat, which.deriv.ind=1, cont=c(25,50,75), abs.cont, display="slice",
     zlab="Density derivative function", ...)
```

Value

Plots for 1-d and 2-d are sent to graphics window. Plot for 3-d is sent to RGL window.

In addition to the display options inherited from `plot.kde`, the first derivative has `display="quiver"`. This is a quiver plot where the size and direction of the arrow indicates the magnitude/direction of the density gradient. See `quiver2D` from the **OceanView** package for more details.

See Also

[plot.kde](#)

Examples

```
## univariate example
data(tempb)
fhat1 <- kdde(x=tempb[, "tmin"], deriv.order=1) ## gradient [df/dx, df/dy]
plot(fhat1, xlab="Min. temp.")                ## df/dx
points(20, predict(fhat1, x=20))

## bivariate example
fhat1 <- kdde(x=tempb[, c("tmin", "tmax")], deriv.order=1)
plot(fhat1, display="quiver")
## gradient [df/dx, df/dy]

fhat2 <- kdde(x=tempb[, c("tmin", "tmax")], deriv.order=2)
plot(fhat2, which.deriv.ind=2, display="persp", phi=15)
plot(fhat2, which.deriv.ind=2, display="filled.contour", col.fun=topo.colors)
## d^2 f/(dx dy): purple=-ve, green=zero, beige=+ve
s2 <- kcurv(fhat2)
plot(s2, display="filled.contour")
## summary curvature
```

plot.kde

Plot for kernel density estimate

Description

Plot for kernel density estimate for 1- to 3-dimensional data.

Usage

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

Arguments

`x` an object of class `kde` (output from [kde](#))

`...` other graphics parameters:

`display` type of display, "slice" for contour plot, "persp" for perspective plot, "image" for image plot, "filled.contour" for filled contour plot (1st form), "filled.contour2" (2nd form) (2-d)

`cont` vector of percentages for contour level curves

`abs.cont` vector of absolute density estimate heights for contour level curves

`approx.cont` flag to compute approximate contour levels. Default is FALSE.

`col` plotting colour for density estimate (1-d, 2-d)

`col.cont` plotting colour for contours

`col.fun` plotting colour function for contours

`col.pt` plotting colour for data points

`colors` vector of colours for each contour (3-d)

`jitter` flag to jitter rug plot (1-d). Default is TRUE.

`lwd.fc` line width for filled contours (2-d)

`xlim,ylim,zlim` axes limits

`xlab,ylab,zlab` axes labels

`add` flag to add to current plot. Default is FALSE.

`theta,phi,d,border` graphics parameters for perspective plots (2-d)

`drawpoints` flag to draw data points on density estimate. Default is FALSE.

`drawlabels` flag to draw contour labels (2-d). Default is TRUE.

`alpha` transparency value of plotting symbol (3-d)

`alphavec` vector of transparency values for contours (3-d)

`size` size of plotting symbol (3-d).

Details

For kde objects, the function headers for the different dimensional data are

```
## univariate
plot(fhat, xlab, ylab="Density function", add=FALSE, drawpoints=FALSE,
     col.pt="blue", col.cont=1, cont.lwd=1, jitter=FALSE, cont, abs.cont,
     approx.cont=TRUE, ...)

## bivariate
plot(fhat, display="slice", cont=c(25,50,75), abs.cont, approx.cont=TRUE,
     xlab, ylab, zlab="Density function", cex=1, pch=1, add=FALSE,
     drawpoints=FALSE, drawlabels=TRUE, theta=-30, phi=40, d=4, col.pt="blue",
     col, col.fun, lwd=1, border=1, thin=3, lwd.fc=5, ...)

## trivariate
plot(fhat, cont=c(25,50,75), abs.cont, approx.cont=FALSE, colors,
     add=FALSE, drawpoints=FALSE, alpha, alphavec, xlab, ylab, zlab,
     size=3, col.pt="blue", ...)
```

The 1-d plot is a standard plot of a 1-d curve. If `drawpoints=TRUE` then a rug plot is added. If `cont` is specified, the horizontal line on the x-axis indicates the `cont%` highest density level set.

There are different types of plotting displays for 2-d data available, controlled by the `display` parameter. (a) If `display="slice"` then a slice/contour plot is generated using `contour`. (b) If `display` is `"filled.contour"` or `"filled.contour2"` then a filled contour plot is generated. The default contours are at 25%, 50%, 75% or `cont=c(25, 50, 75)` which are upper percentages of highest density regions. (c) If `display="persp"` then a perspective/wire-frame plot is generated. The default z-axis limits `zlim` are the default from the usual `persp` command. (d) If `display="image"` then an image plot is generated. Default colours are the default from the usual `image` command.

For 3-dimensional data, the interactive plot is a series of nested 3-d contours. The default contours are `cont=c(25, 50, 75)`. The default colors are `heat.colors` and the default opacity `alphavec` ranges from 0.1 to 0.5.

To specify contours, either one of `cont` or `abs.cont` is required. `cont` specifies upper percentages which correspond to probability contour regions. If `abs.cont` is set to particular values, then contours at these levels are drawn. This second option is useful for plotting multiple density estimates with common contour levels. See [contourLevels](#) for details on computing contour levels. If `approx=FALSE`, then the exact KDE is computed. Otherwise it is interpolated from an existing KDE grid. This can dramatically reduce computation time for large data sets.

Value

Plots for 1-d and 2-d are sent to graphics window. Plot for 3-d is sent to RGL window.

Examples

```
library(MASS)
data(iris)
```

```
## univariate example
fhat <- kde(x=iris[,2])
plot(fhat, cont=50, col.cont="blue", cont.lwd=2, xlab="Sepal length")

## bivariate example
fhat <- kde(x=iris[,2:3])
plot(fhat, display="filled.contour", cont=seq(10,90,by=10))
plot(fhat, display="persp", thin=3, border=1, col="white")

## trivariate example
fhat <- kde(x=iris[,2:4])
plot(fhat, drawpoints=TRUE)
```

plot.kde.loctest *Plot for kernel local significant difference regions*

Description

Plot for kernel local significant difference regions for 1- to 3-dimensional data.

Usage

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

Arguments

x	an object of class <code>kde.loctest</code> (output from <code>kde.local.test</code>)
...	other graphics parameters:
lcol	colour for KDE curve (1-d)
col	vector of 2 colours. Default is <code>c("purple", "darkgreen")</code> . First colour: sample 1>sample 2, second colour: sample 1<sample2.
add	flag to add to current plot. Default is <code>FALSE</code> .
rugsize	height of rug-like plot (1-d)
add.legend	flag to add legend. Default is <code>FALSE</code> (1-d, 2-d).
pos.legend	position label for legend (1-d, 2-d)
add.contour	flag to add contour lines. Default is <code>FALSE</code> (2-d).
	and those used in <code>plot.kde</code>

Details

For `kde.loctest` objects, the function headers are

```
## univariate
plot(x, lcol, col, add=FALSE, xlab="x", ylab, rugsize, add.legend=TRUE,
     pos.legend="topright", ...)
```

```
## bivariate
plot(x, col, add=FALSE, xlab="x", ylab="y", add.contour=FALSE,
     add.legend=TRUE, pos.legend="topright", ...)

## trivariate
plot(x, col, add=FALSE, xlab="x", ylab="y", zlab="z", box=TRUE, axes=TRUE,
     alphavec=c(0.5, 0.5), ...)
```

Value

Plots for 1-d and 2-d are sent to graphics window. Plot for 3-d is sent to RGL window.

See Also

[kde.local.test](#)

Examples

```
library(MASS)
data(crabs)
x1 <- crabs[crabs$sp=="B", c(4,6)]
x2 <- crabs[crabs$sp=="O", c(4,6)]
loct <- kde.local.test(x1=x1, x2=x2)
plot(loct)
```

plot.kde.part

Partition plot for kernel density clustering

Description

Plot of partition for kernel density clustering for 2-dimensional data.

Usage

```
mvnorm.mixt.part(mus, Sigmas, props=1, xmin, xmax, gridsize, max.iter=100,
                 verbose=FALSE)
kms.part(x, H, xmin, xmax, gridsize, verbose=FALSE, ...)

## S3 method for class 'kde.part'
plot(x, display="filled.contour", col, add=FALSE, ...)
```

Arguments

mus	(stacked) matrix of mean vectors
Sigmas	(stacked) matrix of variance matrices
props	vector of mixing proportions
xmin, xmax	vector of minimum/maximum values for grid
gridsize	vector of number of grid points
max.iter	maximum number of iterations
verbose	flag to print out progress information. Default is FALSE.
x	matrix of data values or an object of class kde.part
H	bandwidth matrix. If missing, Hpi(x,deriv,order=1) is called by default.
display	type of display, "slice" for contour plot, "persp" for perspective plot, "image" for image plot, "filled.contour" for filled contour plot (1st form), "filled.contour2" (2nd form)
col	vector of plotting colours
add	flag to add to current plot. Default is FALSE.
...	other parameters

Details

For 2-d data, kms.part and mvnorm.mixt.part produces a kde.part object whose values are the class labels, rather than probability density values.

Value

A kernel partition is an object of class kde.part which is a list with fields:

x	data points - same as input
eval.points	vector or list of points at which the estimate is evaluated
estimate	density estimate at eval.points
H	bandwidth matrix
gridtype	"linear"
gridded	flag for estimation on a grid
binned	flag for binned estimation
names	variable names
w	weights
cont	probability contour levels (if compute.cont=TRUE)
end.points	matrix of final iterates starting from x
label	vector of cluster labels
mode	matrix of cluster modes
nclust	number of clusters
nclust.table	frequency table of cluster labels
tol.iter, tol.clust, min.clust.size	tuning parameter values - same as input

Plot is sent to graphics window.

See Also[plot.kde](#), [kms](#)**Examples**

```
## normal mixture partition
mus <- rbind(c(-1,0), c(1, 2/sqrt(3)), c(1,-2/sqrt(3)))
Sigmas <- 1/25*rbind(invvech(c(9, 63/10, 49/4)), invvech(c(9,0,49/4)), invvech(c(9,0,49/4)))
props <- c(3,3,1)/7
nmixt.part <- mvnorm.mixt.part(mus=mus, Sigmas=Sigmas, props=props)
plot(nmixt.part, asp=1, xlim=c(-3,3), ylim=c(-3,3))

## Not run:
## kernel mean shift partition
set.seed(81928192)
x <- rmvnorm.mixt(n=1000, mus=mus, Sigmas=Sigmas, props=props)
msize <- round(151^2*0.05)
kms.nmixt.part <- kms.part(x=x, min.clust.size=msize)
plot(kms.nmixt.part, asp=1, xlim=c(-3,3), ylim=c(-3,3))
## End(Not run)
```

plot.kfs

*Plot for kernel feature significance***Description**

Plot for kernel significant regions for 1- to 3-dimensional data.

Usage

```
## S3 method for class 'kfs'
plot(x, display="filled.contour", col="orange", colors="orange", abs.cont,
      alphavec=0.4, add=FALSE, ...)
```

Arguments

x	an object of class kfs (output from kfs)
display	type of display, "slice" for contour plot, "persp" for perspective plot, "image" for image plot, "filled.contour" for filled contour plot (1st form), "filled.contour2" (2nd form) (2-d)
col, colors	colour for contour region (1-d, 2-d), (3-d)
abs.cont	absolute contour height. Default is 0.5.
alphavec	transparency value for contour (3-d)
add	flag to add to current plot. Default is FALSE.
...	other graphics parameters used in plot.kde

Value

Plots for 1-d and 2-d are sent to graphics window. Plot for 3-d is sent to RGL window.

See Also

[plot.kde](#)

Examples

```
library(MASS)
data(geyser)
geyser.fs <- kfs(geyser, binned=TRUE)
plot(geyser.fs)
```

plot.kroc

Plot for kernel receiver operating characteristic curve (ROC) estimate

Description

Plot for kernel receiver operating characteristic curve (ROC) estimate 1- to 3-dimensional data.

Usage

```
## S3 method for class 'kroc'
plot(x, add=FALSE, add.roc.ref=FALSE, ylab, xlab, ...)
```

Arguments

x	an object of class kroc (output from kroc)
add	flag to add to current plot. Default is FALSE.
add.roc.ref	flag to add reference ROC curve. Default is FALSE.
xlab	x-axis label. Default is "False positive rate (bar(specificity))".
ylab	y-axis label. Default is "True positive rate (sensitivity)".
...	other graphics parameters used in plot.kde .

Value

Plots for 1-d and 2-d are sent to graphics window. Plot for 3-d is sent to RGL window.

See Also

[plot.kde](#)

Examples

```

library(MASS)
data(fgl)
x1 <- fgl[fgl[,"type"]=="WinF",c("RI", "Na")]
x2 <- fgl[fgl[,"type"]=="Head",c("RI", "Na")]
Rhat <- kroc(x1=x1, x2=x2)
plot(Rhat, add.roc.ref=TRUE)

```

plotmixt

Plot for 1- to 3-dimensional normal and t-mixture density functions

Description

Plot for 1- to 3-dimensional normal and t-mixture density functions.

Usage

```

plotmixt(mus, sigmas, Sigmas, props, dfs, dist="normal", draw=TRUE,
         deriv.order=0, which.deriv.ind=1, binned=TRUE, ...)

```

Arguments

mus	(stacked) matrix of mean vectors
sigmas	vector of standard deviations (1-d)
Sigmas	(stacked) matrix of variance matrices (2-d, 3-d)
props	vector of mixing proportions
dfs	vector of degrees of freedom
dist	"normal" - normal mixture, "t" - t-mixture
draw	flag to draw plot. Default is TRUE.
deriv.order	derivative order
which.deriv.ind	index of which partial derivative to plot
binned	flag for binned estimation of contour levels. Default is TRUE.
...	other graphics parameters, see plot.kde

Value

If draw=TRUE, the 1-d, 2-d plot is sent to graphics window, 3-d plot to RGL window. If draw=FALSE, then a kdde-like object is returned.

Examples

```
## bivariate
mus <- rbind(c(0,0), c(-1,1))
Sigma <- matrix(c(1, 0.7, 0.7, 1), nr=2, nc=2)
Sigmas <- rbind(Sigma, Sigma)
props <- c(1/2, 1/2)
plotmixt(mus=mus, Sigmas=Sigmas, props=props, display="filled.contour")

## trivariate
mus <- rbind(c(0,0,0), c(-1,0.5,1.5))
Sigma <- matrix(c(1, 0.7, 0.7, 0.7, 1, 0.7, 0.7, 0.7, 1), nr=3, nc=3)
Sigmas <- rbind(Sigma, Sigma)
props <- c(1/2, 1/2)
plotmixt(mus=mus, Sigmas=Sigmas, props=props, dfs=c(11,8), dist="t")
```

pre.transform

Pre-sphering and pre-scaling

Description

Pre-sphered or pre-scaled version of data.

Usage

```
pre.sphere(x, mean.centred=FALSE)
pre.scale(x, mean.centred=FALSE)
```

Arguments

`x` matrix of data values
`mean.centred` flag to centre the data values to have zero mean. Default is FALSE.

Details

For pre-scaling, the data values are pre-multiplied by $\mathbf{S}^{-1/2}$ and for pre-sphering, by $\mathbf{S}_D^{-1/2}$ where \mathbf{S} is the sample variance and \mathbf{S}_D is $\text{diag}(S_1^2, S_2^2, \dots, S_d^2)$ where S_i^2 is the i -th marginal sample variance.

Value

Pre-sphered or pre-scaled version of data. These pre-transformations are required for implementing the plug-in [Hpi](#) selectors and the smoothed cross validation [Hscv](#) selectors.

Examples

```
data(unicef)
unicef.sp <- pre.sphere(as.matrix(unicef))
```

quake	<i>Geographical locations of earthquakes</i>
-------	--

Description

The quake data set contains the geographical locations of severe earthquakes in the years 100 and 2016 inclusive. The plate data set contains the geographical locations of the tectonic plate boundaries.

Usage

```
data(quake)
data(plate)
```

Format

–For quake, a matrix with 5871 rows and 5 columns. Each row corresponds to an earthquake. The first column is the year (negative years indicate B.C.E.), the second is the longitude (decimal degrees), the third is the latitude (decimal degrees), the fourth is the depth beneath the Earth’s surface (km), the fifth is a flag for the location inside the circum-Pacific belt (aka Pacific Ring of Fire).

–For plate, a matrix with 3 columns and 6276 rows. Each row corresponds to an location of the tectonic plate boundaries. The first is the longitude, the second is the latitude, the third is the label of the tectonic plate.

Source

Bird, P. (2003) An updated digital model of plate boundaries, *Geochemistry, Geophysics, Geosystems* **4(3)**, 1-52. 1027.

NGDC/WDS (2017) Global significant earthquake database, National Geophysical Data Center, NOAA, doi:10.7289/V5TD9V7K. National Geophysical Data Center/World Data Service. Accessed 2017-03-30.

rkde	<i>Derived quantities from kernel density estimates</i>
------	---

Description

Derived quantities from kernel density estimates.

Usage

```
dkde(x, fhat)
pkde(q, fhat)
qkde(p, fhat)
rkde(n, fhat, positive=FALSE)
```

Arguments

x, q	vector of quantiles
p	vector of probabilities
n	number of observations
positive	flag to compute KDE on the positive real line. Default is FALSE.
fhat	kernel density estimate, object of class kde

Details

pkde uses Simpson's rule for the numerical integration. rkde uses Silverman (1986)'s method to generate a random sample from a KDE.

Value

For the 1-d kernel density estimate fhat, pkde computes the cumulative probability for the quantile q, qkde computes the quantile corresponding to the probability p.

For any kernel density estimate, dkde computes the density value at x (it is an alias for predict.kde), rkde computes a random sample of size n.

References

Silverman, B. (1986) *Density Estimation for Statistics and Data Analysis*. Chapman & Hall/CRC. London.

Examples

```
set.seed(8192)
x <- rnorm.mixt(n=10000, mus=0, sigmas=1, props=1)
fhat <- kde(x=x, binned=TRUE)
p1 <- pkde(fhat=fhat, q=c(-1, 0, 0.5))
qkde(fhat=fhat, p=p1)
y <- rkde(fhat=fhat, n=100)

x <- rmvnorm.mixt(n=10000, mus=c(0,0), Sigmas=invvech(c(1,0.8,1)))
fhat <- kde(x=x, binned=TRUE)
y <- rkde(fhat=fhat, n=1000)
fhaty <- kde(x=y, binned=TRUE)
plot(fhat)
plot(fhaty, add=TRUE, col=2)
```

tempb	<i>Daily temperature</i>
-------	--------------------------

Description

This data set contains the daily minimum and maximum temperatures from the weather station in Badajoz, Spain, from 1 January 1955 to 31 December 2015.

Usage

data(hsct)

Format

A matrix with 21908 rows and 5 columns. Each row corresponds to a daily measurement. The first column is the year (yyyy), the second is the month (mm), the third is the day (dd), the fourth is the minimum temperature (degrees Celsius), the fifth is the maximum temperature (degrees Celsius).

Source

Menne, M. J., Durre, I., Vose, R. S., Gleason, B. E. & Houston, T. (2012) An overview of the global historical climatology network-daily database, *Journal of Atmospheric and Oceanic Technology* **429**, 897 - 910. <https://climexp.knmi.nl/selectdailyseries.cgi>. Accessed 2016-10-20.

unicef	<i>Unicef child mortality - life expectancy data</i>
--------	--

Description

This data set contains the number of deaths of children under 5 years of age per 1000 live births and the average life expectancy (in years) at birth for 73 countries with GNI (Gross National Income) less than 1000 US dollars per annum per capita.

Usage

data(unicef)

Format

A matrix with 2 columns and 73 rows. Each row corresponds to a country. The first column is the under 5 mortality rate and the second is the average life expectancy.

Source

Unicef (2003). *State of the World's Children Report 2003*, Oxford University Press, for Unicef.

vector *Vector and vector half operators*

Description

The `vec` (vector) operator takes a $d \times d$ matrix and stacks the columns into a single vector of length d^2 . The `vech` (vector half) operator takes a symmetric $d \times d$ matrix and stacks the lower triangular half into a single vector of length $d(d+1)/2$. The functions `invvec` and `invvech` are the inverses of `vec` and `vech` i.e. they form matrices from vectors.

Usage

```
vec(x, byrow=FALSE)
vech(x)
invvec(x, ncol, nrow, byrow=FALSE)
invvech(x)
```

Arguments

<code>x</code>	vector or matrix
<code>ncol, nrow</code>	number of columns and rows for inverse of <code>vech</code>
<code>byrow</code>	flag for stacking row-wise or column-wise. Default is FALSE.

References

Magnus, J.R. & Neudecker H.M. (1999) *Matrix Differential Calculus with Applications in Statistics and Econometrics (revised edition)*, Wiley & Sons. Chichester.

Examples

```
x <- matrix(1:9, nrow=3, ncol=3)
vec(x)
invvec(vec(x))
```

vkde *Variable kernel density estimate.*

Description

Variable kernel density estimate for 2-dimensional data.

Usage

```
kde.balloon(x, H, h, gridsize, gridtype, xmin, xmax, supp=3.7, eval.points,
  binned, bgridsize, w, compute.cont=TRUE, approx.cont=TRUE, verbose=FALSE)
kde.sp(x, H, h, gridsize, gridtype, xmin, xmax, supp=3.7, eval.points,
  binned, bgridsize, w, compute.cont=TRUE, approx.cont=TRUE, verbose=FALSE)
```

Arguments

x	matrix of data values
H	bandwidth matrix. If this missing, Hns is called by default.
h	not yet implemented
gridsize	vector of number of grid points
gridtype	not yet implemented
xmin, xmax	vector of minimum/maximum values for grid
supp	effective support for standard normal
eval.points	vector or matrix of points at which estimate is evaluated
binned	flag for binned estimation.
bgridsize	vector of binning grid sizes
w	vector of weights. Default is a vector of all ones.
compute.cont	flag for computing 1% to 99% probability contour levels. Default is TRUE.
approx.cont	flag for computing approximate probability contour levels. Default is TRUE.
verbose	flag to print out progress information. Default is FALSE.

Details

The balloon density estimate `kde.balloon` employs bandwidths which vary at each estimation point (Loftsgaarden & Quesenberry, 1965). There are as many bandwidths as there are estimation grid points. The default bandwidth is `Hns(,deriv.order=2)` and the subsequent bandwidths are derived via a minimal MSE formula.

The sample point density estimate `kde.sp` employs bandwidths which vary for each data point (Abramson, 1982). There are as many bandwidths as there are data points. The default bandwidth is `Hns(,deriv.order=4)` and the subsequent bandwidths are derived via the Abramson formula.

Value

A variable kernel density estimate for bounded data is an object of class `kde`.

References

Abramson, I. S. (1982) On bandwidth variation in kernel estimates - a square root law. *Annals of Statistics*, **10**, 1217-1223.

Loftsgaarden, D. O. & Quesenberry, C. P. (1965) A nonparametric estimate of a multivariate density function. *Annals of Mathematical Statistics*, **36**, 1049-1051.

See Also

[kde](#), [plot.kde](#)

Examples

```
data(worldbank)
wb <- as.matrix(na.omit(worldbank[,4:5]))
xmin <- c(-70,-25); xmax <- c(25,70)
fhat <- kde(x=wb, xmin=xmin, xmax=xmax)
fhat.sp <- kde.sp(x=wb, xmin=xmin, xmax=xmax)
plot(fhat, display="persp", box=TRUE, phi=20, zlim=c(0,max(fhat.sp$estimate)))
plot(fhat.sp, display="persp", box=TRUE, phi=20, zlim=c(0,max(fhat.sp$estimate)))
## Not run:
fhat.ball <- kde.balloon(x=wb, xmin=xmin, xmax=xmax)
plot(fhat.ball, display="persp", box=TRUE, phi=20, zlim=c(0,max(fhat.sp$estimate)))
## End(Not run)
```

worldbank

Development indicators from the World Bank Group

Description

This data set contains six development indicators for national entities for the year 2011, which is the latest year for which they are consistently available.

Usage

```
data(worldbank)
```

Format

A matrix with 7 columns and 218 rows. Each row corresponds to a country. The first column is the country, the second is the per capita carbon dioxide emissions (thousands Kg), the third is the per capita GDP (thousands of current USD), the fourth is the annual GDP growth rate (%), the fifth is the annual inflation rate (%), the sixth is the percentage of internet users in the population (%), the seventh is the added value agricultural production as a ratio of the total GDP (%).

Source

World Bank Group (2016) World development indicators. <http://databank.worldbank.org/data/reports.aspx?source=world-development-indicators>. Accessed 2016-10-03.

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