# Package ‘LPCM’

September 22, 2015

**Type** Package  
**Title** Local Principal Curve Methods  
**Version** 0.45-0  
**Date** 2015-09-21  
**Author** Jochen Einbeck and Ludger Evers  
**Maintainer** Jochen Einbeck <jochen.einbeck@durham.ac.uk>  
**Depends** R (>= 2.10)  
**Suggests** scatterplot3d, lattice, dr  
**Description** Fitting multivariate data patterns with local principal curves; including simple tools for data compression (projection), bandwidth selection, and measuring goodness-of-fit.  
**License** GPL (>= 2)  
**LazyLoad** yes  
**NeedsCompilation** no  
**Repository** CRAN  
**Date/Publication** 2015-09-22 13:00:32

## R topics documented:

<table>
<thead>
<tr>
<th>Topic</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>LPCM-package</td>
<td>2</td>
</tr>
<tr>
<td>calspeedflow</td>
<td>3</td>
</tr>
<tr>
<td>coverage</td>
<td>4</td>
</tr>
<tr>
<td>followx</td>
<td>7</td>
</tr>
<tr>
<td>gaia</td>
<td>8</td>
</tr>
<tr>
<td>gvessel</td>
<td>10</td>
</tr>
<tr>
<td>kernels.and.distances</td>
<td>11</td>
</tr>
<tr>
<td>lpc</td>
<td>12</td>
</tr>
<tr>
<td>lpc.control</td>
<td>14</td>
</tr>
<tr>
<td>lpc.project</td>
<td>16</td>
</tr>
<tr>
<td>lpc.spline</td>
<td>17</td>
</tr>
<tr>
<td>lpc.spline.auxiliary.functions</td>
<td>19</td>
</tr>
<tr>
<td>ms</td>
<td>20</td>
</tr>
</tbody>
</table>
Description

Fitting multivariate data patterns with local principal curves; including simple tools for data compression (projection), bandwidth selection, and measuring goodness-of-fit.

This package implements the techniques introduced in Einbeck, Tutz & Evers (2005), and successive related papers.

The main functions to be called by the user are

- `lpc`, for the estimation of the local centers of mass which make up the principal curve;
- `lpc.spline`, which is a smooth and fully parametrized cubic spline representation of the latter;
- `lpc.project`, which enables to compress data by projecting them orthogonally onto the curve;
- `lpc.coverage` and `Rc` for assessing goodness-of-fit;
- `lpc.self.coverage` for bandwidth selection;
- the generic `plot` and `print` methods for objects of class `lpc` and `lpc.spline`.

This package also contains some code for density mode detection ('local principal points') and mean shift clustering (as well as bandwidth selection in this context), which implements the methods presented in Einbeck (2011). See the help file for `ms`.

A second R package which will implement the extension of local principal curves to local principal surfaces and manifolds, as proposed in Einbeck, Evers & Powell (2010), is in preparation.

Details

- Package: LPCM
- Type: Package
- License: GPL (>=2)
- LazyLoad: yes
Acknowledgements
Contributions (in form of pieces of code, or useful suggestions for improvements) by Jo Dwyer, Mohammad Zayed, and Ben Oakley are gratefully acknowledged.

Author(s)
Jochen Einbeck and Ludger Evers
Maintainer: Jochen Einbeck <jochen.einbeck@durham.ac.uk>

References

See Also
pcurve, princurve

Description
A ‘fundamental diagram’ with observations of speed and flow recorded from 9th of July 2007, 9am, to 10th of July 2007, 10pm, on Line 5 of the Californian Freeway SR57-N, VDS number 1202263. The data were originally measured in intervals of thirty seconds, and then aggregated over intervals of 5 minutes length.

Usage
data(calspeedflow)

Format
A data frame with 444 observations on the following 4 variables.
Date a factor with levels 07/09/2007... 07/10/2007.
Timestamp a factor with timestamps in intervals of five minutes.
Lane5Flow a numeric vector of vehicle flow in vehicles per 5 minutes.
Lane5Speed a numeric vector of vehicle speed in miles per hour.
Source
Retrieved from PeMS.

References

Examples
data(calspeedflow)
plot(calspeedflow[,3:4])

coverage

Coverage and self-coverage plots.

Description
These functions compute coverages (for any principal object), and self-coverages (only for local principal curves, these may be used for bandwidth selection).

Usage

coverage.raw(X, vec, tau, weights=1, plot.type="p", print=FALSE, label= NULL, ...)

coverage(X, vec, tau.min=0.02, tau.max=25, gridsize=25, weights=1, plot.type="o", print=FALSE, ...)

lpc.coverage(object, tau.min=0.02, tau.max, gridsize=25, quick=TRUE, plot.type="o", print=FALSE, ...)

lpc.self.coverage(X, tau.min=0.02, tau.max=0.5, gridsize=25, x0=1, way="two", scaled=TRUE, weights=1, pen=2, depth=1, control=lpc.control(boundary=0, cross=FALSE), quick=TRUE, plot.type="o", print=FALSE, ...)

select.self.coverage(self, smin, plot.type="o", plot.segments=NULL)

Arguments

X
object
vec
tau

a $N \times d$ data matrix.
An object of type lpc or lpc.spline.
A matrix with $d$ columns. The rows contain the points which make up the fitted object.
tube size.
coverage

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>taumin</td>
<td>Minimal tube size.</td>
</tr>
<tr>
<td>taumax</td>
<td>Maximal tube size.</td>
</tr>
<tr>
<td>weights</td>
<td>An optional vector of weights. If weights are specified, then the coverage is the weighted mean of the indicator functions for falling within the tube. The function <code>lpc.coverage</code> does not have a <code>weights</code> argument, as it extracts the weights from the <code>weights</code> component of the fitted object.</td>
</tr>
<tr>
<td>label</td>
<td>Experimental option; don’t use.</td>
</tr>
<tr>
<td>gridsize</td>
<td>The number of different tube sizes to consider.</td>
</tr>
<tr>
<td>quick</td>
<td>If TRUE, an approximate coverage curve is provided by computing distances between data points and the curve through the closest local centers or mass; whereas with FALSE we use the distances of the points when projected orthogonally onto the spline representation of the local principal curve. The latter takes considerably more computing time. The resulting coverage curves are generally very similar, but the quick version may deliver little spurious peaks occasionally.</td>
</tr>
<tr>
<td>self</td>
<td>An object of class <code>self</code>, or a matrix with two columns providing a self-coverage curve.</td>
</tr>
<tr>
<td>smin</td>
<td>Minimum coverage for bandwidth selection. Default: 1/3 for clustering, 2/3 for principal curves.</td>
</tr>
<tr>
<td>plot.type</td>
<td>If set to 0, no plotted output is given. Otherwise, an appropriate plot is provided, using the plotting type as specified.</td>
</tr>
<tr>
<td>plot.segments</td>
<td>A list with default <code>list(lty=c(1,2,3), lwd=c(2,1,1), lcol=c(3,3,3))</code> which specifies how (and how many) bandwidth candidates, in order of decreasing negative second derivative of self-coverage, are to be highlighted.</td>
</tr>
<tr>
<td>print</td>
<td>If TRUE, coverage values are printed on the screen as soon as computed. This is quite helpful especially if <code>gridsize</code> is large.</td>
</tr>
<tr>
<td>x0, way, scaled, pen, depth, control</td>
<td>LPC parameters as outlined in <code>lpc</code> and <code>lpc.control</code>.</td>
</tr>
<tr>
<td>...</td>
<td>Optional graphical parameters passed to the corresponding plotting functions.</td>
</tr>
</tbody>
</table>

Details

The function `coverage.raw` computes the coverage, i.e. the proportion of data points lying inside a circle or band with radius \( \tau \), for a fixed value `tau`. The whole coverage curve \( C(\tau) \) is constructed through function `coverage`.

Functions `coverage.raw` and `coverage` can be used for any object fitted by an unsupervised learning technique (for instance, HS principal curves, or even clustering algorithms), while the functions prefixing with `lpc` can only be used for local principal curves. The function `lpc.coverage` is a wrapper around `coverage` which takes directly a fitted `lpc` object, rather than a data matrix.

Function `select.self.coverage` extracts suitable bandwidths from the self-coverage curve, and produces a plot. The function is called from within `lpc.self.coverage`, but can also be called directly by the user (for instance, if the graphical output is to be reproduced, or if the minimum coverage `smin` is to be modified). The component `$select` contains the selected candidate bandwidths, in the order of strength of evidence provided by the self-coverage criterion (the best bandwidth comes first, etc.). A plot is produced as a by-product, which symbolizes the best bandwidth by a thick solid.
line, the second-best by a dashed line, and the third-best by a dotted line. It is recommended to run the self-coverage functions with fixed starting points, as in the examples below.

See Einbeck (2011) for details. Note that the original publication by Einbeck, Tutz, and Evers (2005) uses ‘quick’ coverage curves.

Value

A list of items, and a plot (unless plot.type=0).

The function lpc.self.coverage produces an object of class self. The component $select recommends suitable bandwidths for the use in lpc, in the order of strength of evidence. These correspond to points of strong negative curvature (implemented via second differences) of the self-coverage curve.

Author(s)

J. Einbeck

References


See Also

lpc

Examples

data(gvessel)
## Not run: gvessel.self <- lpc.self.coverage(gvessel[,c(2,4,5)], x0=c(35, 1870, 6.3), print=FALSE, plot.type=0)
h <- select.self.coverage(gvessel.self)$select
gvessel.lpc <- lpc(gvessel[,c(2,4,5)], h=h[1], x0=c(35, 1870, 6.3))
lpc.coverage(gvessel.lpc, gridsize=10, print=FALSE)

## End(Not run)

data(calspeedflow)
fitms <- ms(calspeedflow[,3:4])
coverage(fitms$data, fitms$cluster.center)
followx

Fit an individual branch of a local principal curve.

Description

Internal function of package LPCM called by lpc. Do not use!

Usage

followx(Xi, x0, h, t0, iter, way, weights, pen = 2, phi = 1, 
lasteigenvector = 0, rho0 = 0.4, boundary=0.005, 
convergence.at= 0.000001, cross=TRUE)

Arguments

Xi
x0
h
t0
iter
way
weights
pen
phi
lasteigenvector
rho0
boundary
convergence.at
cross

Author(s)

JE

See Also

lpc
Description

(Simulated) spectral decomposition of stellar objects, generated in the framework of the Gaia project.

Usage

data(gaia)

Format

A data frame with 8286 observations on the following 22 variables.

ID  ID of the object
metallicity  metallicity (abundance); that is proportion of matter other than hydrogen and helium relative to that of the sun.
gravity  the surface gravity; that is acceleration due to gravity at the surface of the star.
temperature  the ‘effective’ temperature (K); that is the temperature of the observable part of the stellar atmosphere.
band1  photon counts in band 1
band2  photon counts in band 2
band3  photon counts in band 3
band4  photon counts in band 4
band5  photon counts in band 5
band6  photon counts in band 6
band7  photon counts in band 7
band8  photon counts in band 8
band9  photon counts in band 9
band10  photon counts in band 10
band11  photon counts in band 11
band12  photon counts in band 12
band13  photon counts in band 13
band14  photon counts in band 14
band15  photon counts in band 15
band16  photon counts in band 16
Details

Gaia is an astrophysics mission of the European Space Agency (ESA) which will undertake a detailed survey of over $10^9$ stars in our Galaxy and extragalactic objects. An important part of the scientific analysis of these data is the classification of all the objects as well as the estimation of stellar astrophysical parameters (effective stellar temperature, surface gravity, metallicity). This will be done on the basis of high-dimensional spectroscopic and astrometric data such as those ones given here.

More precisely, the spectral data come in form of photon counts (“fluxes”) observed in (originally) 96 wavelength intervals (“bands”), see Bailer-Jones (2010) for more details. The data given here are a 16-dimensional subset created by binning/selecting from the 96 bands. The counts given here are standardized, i.e. they are divided by the total number of incoming photons over all filters (in other words, they add up to 1). Note that these data are simulated using computer models. The satellite which will collect the actual data will be launched in 2012.

The 16-d spectral data have been used in Einbeck, Evers and Bailer-Jones (2008) as well as Einbeck, Evers and Powell (2010) in order to predict the stellar temperature.

Source

Coryn Bailer-Jones (MPIA Heidelberg).

References


Examples

data(gaia)
s <- sample(nrow(gaia),200)
library(lattice)
splom(gaia[,5:20], cex=0.3, pscales=0)

gaia.pc <- princomp(gaia[,5:20])
temp <- gaia$temperature
tempcol <- (temp[- min(temp)]/max(temp[- min(temp)]))
library(scatterplot3d)
scatterplot3d(gaia.pc$scores[, c(2,1,3)], pch="+", color=rgb(sqrt(tempcol),0,1-sqrt(tempcol)))
   # This is a 3D scatterplot of the first three principal component scores;
   # with higher stellar temperatures shaded in red colour.
gvessel

North Atlantic Water Temperature Data.

Description

These are observations taken over nine days in May 2000 by the German vessel Gauss in the North Atlantic.

Usage

data(gvessel)

Format

A data frame with 643 observations on the following 7 variables.

day  an integer for the day at which the measurement was taken.
salg a numeric vector with measurements of salinity according to the PSS (Practical Salinity Scale).
tempg a numeric vector with measurements of water temperature in degrees Celsius.
depthg a numeric vector with the water depths (in meters) at which the measurements were taken.
oxyg a numeric vector with measurements of oxygen content (mm per litre of water)
longg longitude
latg latitude

Source


References


Examples

data(gvessel)
pairs(gvessel[,c(3,2,4,5)])
tcol <- (gvessel$tempg- min(gvessel$tempg))/(max(gvessel$tempg)- min(gvessel$tempg))
require(scatterplot3d)
scatterplot3d(gvessel[,2],gvessel[,4],gvessel[,5], color=rgb(tcol,0,1-tcol))
Auxiliary kernel and distance functions.

Description

Internal LPCM functions which are normally not to be called by the user.

Usage

- `kern(y, x = 0, h = 1)`
- `kernd(X, x, h)`
- `kdex(X, x, h)`
- `distancevector(X, y, d = "euclid", na.rm = TRUE)`
- `vecdist(X,Y)`
- `mindist(X,Y)`
- `enorm(x)`

Arguments

- `x` a number or vector.
- `y` a vector.
- `h` a bandwidth.
- `X` a matrix.
- `Y` a matrix.
- `d` type of distance measure (only 'euclid').
- `na.rm` ...

Details

- `kern` specifies the base kernel (by default Gaussian) used in lpc; `kernd` is the corresponding multivariate product kernel. `kdex` is a pointwise multivariate kernel density estimator.
- `distancevector` makes use of function `vdisseuclid` from R package `hopach` (but that package does not need to be loaded).

Author(s)

JE

References

Description

This is the main function which computes the actual local principal curve, i.e. a sequence of local centers of mass.

Usage

\[ \text{lpc}(X, h, t0 = \text{mean}(h), x0, \ \text{way} = "two", \ \text{scaled} = \text{TRUE}, \ \text{weights}=1, \ \text{pen} = 2, \ \text{depth} = 1, \ \text{control}=\text{lpc.control}()) \]

Arguments

- **X**: data matrix with \(N\) rows (observations) and \(d\) columns (variables).
- **h**: bandwidth. May be either specified as a single number, then the same bandwidth is used in all dimensions, or as a \(d\)-dimensional bandwidth vector. The default setting is 10 percent of the range in each direction. If \text{scaled} = \text{TRUE} then the bandwidth has to be specified in fractions of the data range, e.g. \(h = c(0.2, 0.1)\), rather than absolute values.
- **t0**: scalar step length. Default setting is \(t0 = h\), if \(h\) is a scalar, and \(t0 = \text{mean}(h)\), if \(h\) is a vector.
- **x0**: specifies the choice of starting points. The default choice \(x0 = 1\) will select one suitable starting point automatically (in form of a local density mode). The second built-in option \(x0=0\) will use all local density modes as starting points, hence produce as many branches as modes. Optionally, one can also set one or more starting points manually here. This can be done in form of a matrix, where each row corresponds to a starting point, or in form of a vector, where starting points are read in consecutive order from the entries of the vector. The starting point has always to be specified on the original data scale, even if \text{scaled} = \text{TRUE}. A fixed number of starting points can be enforced through option \text{mult} in \text{lpc.control}.
- **way**: "one": go only in direction of the first local eigenvector, "back": go only in opposite direction, "two": go from starting point in both directions.
- **scaled**: if \text{TRUE}, scales each variable by dividing through its range (see also the Notes section below).
- **weights**: a vector of observation weights (can also be used to exclude individual observations from the computation by setting their weight to zero.)
- **pen**: power used for angle penalization (see [1]). If set to 0, the angle penalization is switched off.
- **depth**: maximum depth of branches (\(\phi_{max}\) in [2]), restricted to the values 1, 2 or 3 (The original LPC branch has depth 1. If, along this curve, a point features a high second local PC, this launches a new starting point, and the resulting branch has depth 2. If, along this branch, a point features a high second local PC, this launches a new starting point, and the resulting branch has depth 3.)
control Additional parameters steering particularly the starting-, boundary-, and convergence behavior of the fitted curve. See \texttt{lpc.control}.

\textbf{Value}

A list of items:

\begin{itemize}
\item \textbf{LPC} The coordinates of the local centers of mass of the fitted principal curve.
\item \textbf{Parametrization} Curve parameters and branch labels for each local center of mass.
\item \textbf{h} The bandwidth used for the curve estimation.
\item \textbf{t0} The constant $t_0$ used for the curve estimation.
\item \textbf{starting.points} The coordinates of the starting point(s) used.
\item \textbf{data} The data frame used for curve estimation.
\item \textbf{scaled} Logical.
\item \textbf{weights} The vector of weights used for curve estimation.
\item \textbf{control} The settings used in \texttt{lpc.control()}
\item \textbf{Misc} Miscellanea.
\end{itemize}

\textbf{Note}

All values provided in the output refer to the scaled data, if \texttt{scaled=TRUE}. Use \texttt{unscale} to convert the results back to the original data scale.

The option \texttt{scaled=TRUE} scales the data by dividing each variable through their range. This differs from the usual scaling through the standard deviation as common for PCA, but we found the algorithm and the default bandwidth selection to work more reliably this way. If you wish to scale by the standard deviation, please do that by feeding the scaled data directly into the \texttt{lpc} function, i.e.
\begin{verbatim}
lpc(sweep(data, 2, sd(data), "/"), h, t0, ..., scaled=FALSE, ...).
\end{verbatim}

\textbf{Author(s)}

J. Einbeck and L. Evers. See \texttt{LPCM-package} for further acknowledgements.

\textbf{References}


Examples

\begin{verbatim}
data(calspeedflow)
lpc1 <- lpc(calspeedflow[,3:4])
plot(lpc1)

data(mussels, package="dr")
lpc2 <- lpc(mussels[-3], x0=as.numeric(mussels[49,-3]), scaled=FALSE)
plot(lpc2, curvecol=2)

data(gaia)
s <- sample(nrow(gaia), 200)
gaia.pc <- princomp(gaia[s,5:20])
lpc3 <- lpc(gaia.pc$scores[,2:1:3], scaled=FALSE)
plot(lpc3, curvecol=2, type=c("curve","mass"))

# Simulated letter 'E' with branched LPC
ex <- c(rep(0,40), seq(0,1,length=20), seq(0,1,length=20), seq(0,1,length=20))
ey <- c(rep(0,20), rep(0,20), rep(1,20), rep(0,20))
sex <- rnorm(100, 0, 0.01); sey <- rnorm(100, 0, 0.01)
sexx <- rnorm(100, 0, 0.1); sey <- rnorm(100, 0, 0.1)
ex1 <- ex+sex; ey1 <- ey+sey
ex2 <- ex+exx; ey2 <- ey+sey
e1 <- cbind(ex1, ey1); e2 <- cbind(ex2, ey2)
lpc.e1 <- lpc(e1, h = c(0.1, 0.1), depth=2, scaled=FALSE)
plot(lpc.e1, type=c("curve","mass", "start"))
\end{verbatim}

\section*{Description}

This function bundles parameters controlling mainly the starting-, convergence-, boundary-, and stopping-behaviour of the local principal curve. It will be used only inside the \texttt{lpc()} function argument.

\section*{Usage}

\begin{verbatim}
lpc.control(iter = 100, cross = TRUE,
boundary = 0.005, convergence.at = 0.00001,
mult = NULL, ms.h = NULL, ms.sub = 30,
pruning.thresh = 0.0, rho0 = 0.4)
\end{verbatim}

\section*{Arguments}

\begin{itemize}
\item \texttt{iter} \hspace{1cm} Maximum number of iterations on either side of the starting point within each branch.
\end{itemize}
Logical parameter. If FALSE, a curve is stopped when it comes too close to another part of itself. Note: Even when cross=FALSE, different branches of the curve (for higher depth or multiple starting points) are still allowed to cross. This option only avoids crossing of each particular branch with itself. Used in the self-coverage functions to avoid overfitting.

This boundary correction [2] reduces the bandwidth adaptively once the relative difference of parameter values between two centers of mass falls below the given threshold. This measure delays convergence and enables the curve to proceed further into the end points. If set to 0, this boundary correction is switched off.

This forces the curve to stop if the relative difference of parameter values between two centers of mass falls below the given threshold. If set to 0, then the curve will always stop after exactly iter iterations.

Numerical value which enforces a fixed number of starting points. If the number given here is larger than the number of starting points provided at x0, then the missing points will be set at random (For example, if \( d = 2, \)mult=3, and \( x0=[58.5, 17.8, 80, 20] \), then one gets the starting points \( [58.5, 17.8], (80, 20) \), and a randomly chosen third one. Another example for such a situation is \( x0=NULL \) with mult=1, in which one random starting point is chosen). If the number given here is smaller than the number of starting points provided at x0, then only the first mult starting points will be used.

Sets the bandwidth (vector) for the initial mean shift procedure which finds the local density modes, and, hence, the starting points for the LPC. If unspecified, the bandwidth used in function lpc is used here too.

Proportion of data points (default=30) which are used to initialize mean shift trajectories for the mode finding. In fact, we use \( \min(\max(\text{ms.sub}, \text{floor}(\text{ms.sub}*N/100)), 10*\text{ms.sub}) \) trajectories.

Prunes branches corresponding to higher-depth starting points if their density estimate falls below this threshold. Typically, a value between 0.0 and 1.0. The setting 0.0 means no pruning.

A numerical value which steers the birth process of higher-depth starting points. Usually, between 0.3 and 0.4 (see reference [1]).

A list of the nine specified input parameters, which can be read by the control argument of the lpc function.

JE


```
data(calspeedflow)
fit1 <- lpc(calspeedflow[,c(3,4)], x0=c(50,60), scaled=TRUE,
          control=lpc.control(iter=20, boundary=0))
plot(fit1, type=c("curve","start","mass"))
```

**Description**

Projects a new observation onto the spline representation of the local principal curve.

**Usage**

```r
lpc.project(object, newdata, ...)
```

**Arguments**

- `object`: Object of class `lpc` or `lpc.spline`.
- `newdata`: A data frame containing the new data to be projected.
- `...`: Additional arguments to be passed to `lpc.project.spline`.

**Value**

- `closest.pi`: Projection index of projected point(s) (in cubic spline parametrization).
- `closest.or.pi`: Projection index of projected point(s) (in terms of the original LPC parametrization).
- `closest.coords`: Coordinates of projected data point(s)
- `closest.dist`: Euclidean distance between data point(s) and their projected counterpart(s).
- `closest.branch`: ID of branch onto which the data point was projected (the IDs get allocated in the output component `$Parameterization` of function `lpc`).

**Note**

The parametrization of the cubic spline function is not exactly the same as that of the original LPC. The reason is that the latter uses Euclidean distances between centers of masses, while the former uses the arc length along the cubic spline. The differences are normally quite small, though.

**Author(s)**

J. Einbeck and L. Evers
References


See Also

lpc, lpc.spline

Examples

data(gvessel)
gvessel.lpc <- lpc(gvessel[,c(2,4,5)], scaled=TRUE, h=0.11, x0=c(35, 1870, 6.3))
lpc.project(gvessel.lpc, newdata=data.frame(salg=35, dephtg= 2000, oxyg=6))

Description

Fits a natural cubic spline component-wise through the series of local centers of mass. This provides a continuous parametrization in terms of arc length distance, which can be used to compute a projection index for the original or new data points.

Usage

lpc.spline(lpcobject, optimize = TRUE, compute.Rc=FALSE, project=FALSE, ...)

Arguments

lpcobject Object of class lpc.
optimize Boolean. If TRUE, optimize is used to find the point on the curve with minimum distance. Otherwise, data points are only projected onto the closest knot.
compute.Rc Boolean. If TRUE, the goodness-of-fit measure $R_C$ suggested in [1] is computed and returned (using the scaled data, if scaled=TRUE in lpcobject).
project Boolean. If TRUE, projections onto curve are computed.
... Additional arguments to be passed to lpc.project.spline

Details

See reference [2].
Value

knots.pi  LPC parameters (in cubic spline parametrization) at position of the knots of the spline function (these are not identical to the LPC mass points!)
knots.coords  Coordinates of the spline knots.
closest.pi  Parameter of the projected data points.
closest.coords  Coordinates of projected data points.
closest.dist  Euclidean distance between original and projected data point.
closest.branch  ID Number of the branch on which the data point was projected (the IDs are given in the output of function lpc).

Rc  Value of $R_C$.
project  repeats the input value of project.
lpcobject  returns the provided object lpcobject.
splinefun  returns the cubic spline function (generated by lpc.splinefun).

Warning

Careful with options project and compute.Rc - they can take rather long if the data set is large!

Note

The parametrization of the cubic spline function is not exactly the same as that of the original LPC. The reason is that the latter uses Euclidean distances between centers of masses, while the former uses the arc length along the cubic spline. However, the differences are normally quite small.

Author(s)

J. Einbeck and L. Evers

References


See Also

lpc

Examples

data(gvessel)
gvessel.lpc <- lpc(gvessel[,c(2,4,5)], h=0.11, x0=c(35, 1870, 6.3))
gvessel.spline <- lpc.spline(gvessel.lpc)
plot(gvessel.spline, lwd=2)
Auxiliary functions for spline fitting and projection.

Description

Internal functions of package LPCM called by lpc.spline and others. These will rarely be called directly by the user.

Usage

lpc.splinefun(lpcobject)

lpc.fit.spline(lpcsl, num.knots = 100)

lpc.spline.eval(lpcsl, or.pi, branch = 0)

lpc.project.spline(lpcsl, newdata, num.knots = 100, optimize = TRUE)

lpc.curve.length(lpcsl, or.pi, branch = 0, total.subdivisions = 10000, min.subdivisions = 100)

Arguments

lpcobject Object of type lpc.
lpcsl Object generated by lpc.splinefun.
num.knots number of spline knots
or.pi original projection index
branch branch ID
newdata new data frame
optimize Boolean.
total.subdivisions total number of subdivisions for arc length computation.
min.subdivisions minimum number of subdivisions for arc length computation.

Author(s)

L. Evers and J. Einbeck

See Also

lpc.spline
Mean shift clustering.

Description

Functions for mean shift, iterative mean shift, mean shift clustering, and bandwidth selection for mean shift clustering (based on self-coverage). The main function is `ms` which, for a given bandwidth, detects the local modes ('local principal points') and performs the clustering.

These functions implement the techniques presented in Einbeck (2011).

Usage

meanshift(X, x, h)
ms.rep(X, x, h, plots=1, thresh= 0.0000001, iter=200)
ms(X, h, subset, thr=0.0001, scaled= TRUE, iter=200, plotms=2,
or.labels=NULL, ...)
ms.self.coverage(X, taumin=0.02, taumax=0.5, gridsize=25,
    thr=0.0001, scaled=TRUE, cluster=FALSE, plot.type="o",
or.labels=NULL, print=FALSE, ...)

Arguments

X data matrix.

h bandwidth (by default, 10 percent of the data range).

x point from which we wish to shift to the local mean.

subset vector specifying a subset of 1:n, where n is the sample size. This allows to run the iterative mean shift procedure only from a subset of points (if unspecified, 1:n is used here, i.e. each data point serves as a starting point).

scaled logical (if TRUE, each variable is divided by its range).

taumin,taumax,gridsize determine the grid of bandwidths to investigate.

thresh, iter mean shift iterations are stopped when the mean shift length (relative to the length of x) falls below thresh, or after iter iterations (whatever event happens first).

thr adjacent mean shift clusters are merged if their relative distance falls below this threshold.

cluster if TRUE, distances are always measured to the cluster to which an observation is assigned, rather than to the nearest cluster.

plotms, plot.type, or.labels, ... graphical parameters.

print if TRUE, coverage values are printed on the screen as soon as computed. This is quite helpful especially if gridsize is large.
**Details**

The methods implemented here can be used for density mode estimation, clustering, and the selection of starting points for the LPC algorithm.

Chen (1995) showed that, if the mean shift is computed iteratively, the resulting sequence of local means converges to a mode of the estimated density function. By assigning each data point to the mode to which it has converged, this turns into a clustering technique.

The concepts of coverage and self-coverage, which were originally introduced in the principal curve context, adapt straightforwardly to this setting.

The goodness-of-fit measure $R_c$ can also be applied in this context. For instance, a value of $R_c = 0.8$ means that, after the clustering, the mean absolute residual length has been reduced by 80% (compared to the distances to the overall mean).

**Value**

The main function `ms` produces an object of class `ms`, with components:

- `cluster.center`: a matrix which gives the coordinates of the estimated density modes (i.e., of the mean-shift based cluster centers).
- `cluster.label`: assigns each data point to the cluster center to which its mean shift trajectory has converged.
- `closest.label`: assigns each data point to the closest cluster center in terms of Euclidean distance.
- `data`: the data frame (scaled if `scaled=TRUE`).
- `scaled`: boolean.
- `scaled.by`: the data were scaled by dividing each variable through the values provided in this vector.

For all other functions, use `names(I)`.

**Author(s)**

J. Einbeck. See LPCM-package for further acknowledgements.

**References**


**See Also**

$R_c$, lpc.self.coverage
Examples

data(faithful)
# Mean shift clustering with user-defined bandwidth (5 percent of data range)
fit <- ms(faithful, h=0.05)

# Goodness-of-fit
coverage(fit$data, fit$cluster.center)
Rc(fit)

# Bandwidth selection via self-coverage
## Not run: foo <- ms.self.coverage(faithful, gridsize= 50, taumin=0.1, taumax=0.5, plot.type="o")
h <- select.self.coverage(foo)$select
fit <- ms(faithful, h=h[1])
## End(Not run)

plot.lpc

Plotting local principal curves

Description

Takes an object of class lpc or lpc.spline and plots any subset of the following components of the local principal curve: Centers of mass; the curve connecting the local centers of mass; the cubic spline representation of the curve; the projections onto the curve; the starting points.

Usage

## S3 method for class 'lpc'
plot(x, type, unscale = TRUE, lwd = 1, datcol = "grey60",
datpch = 21, masscol = NULL, masspch = 15, curvecol = 1, splinecol = 3,
projectcol = 4, startcol = NULL, startpch=NULL,...)

## S3 method for class 'lpc.spline'
plot(x, type, unscale = TRUE, lwd = 1, datcol = "grey60",
datpch = 21, masscol = NULL, masspch = 15, curvecol = 1, splinecol = 3,
projectcol = 4, startcol = NULL, startpch=NULL,...)

Arguments

x an object of class lpc or lpc.spline.
type a vector of type c("mass", "spline",...) with possible entries mass, curve, spline, project, start.
unscale if TRUE, then data (and all fitted componens) are scaled back to their original scale; otherwise the scaled data are plotted (only relevant if scaled=TRUE in the fitted object).
lwd width of curves.
datcol color of data points.
plot.lpc

datpch plotting symbol for data points.

masscol color of centers of mass (see below).

masspch plotting symbol for centers of mass.

curvecol color of the curve interpolating the local centers of mass (this is the "local principal curve"!).

splinecol color of the spline representation of the local principal curve.

projectcol color of projections onto the spline representation of the local principal curve.

startcol color of the plotted starting points.

startpch plotting symbol for starting points; needs to be either a single symbol, or a vector of symbols of the same length as the number of starting points.

... further arguments passed to plot or scatterplot3d.

Value

A 2D plot, 3D plot, or a pairs plot (depending on the data dimension \( d \)).

The most flexible plotting option is \texttt{masscol}. Depending on the length of the specified vector, this will be interpreted differently. If a scalar is provided, the corresponding color will be given to all centers of mass. If the length of the vector is larger than 1, then this option will assign different colours to different depths, or different branch numbers, or to individual data points, depending on the length. The default setting is assigning colours according to depth, in the order red, blue, black.

With increasing dimension \( d \), less plotting options tend to be supported. The nicest plots are obtained for \( d = 2 \) and \( d = 3 \).

Warning

This function computes all missing information (if possible), so computation will take the longer the less informative the given object is, and the more advanced aspects are asked to plot!

Author(s)

JE

References


See Also

\texttt{lpc, lpc.spline}
print.lpc

Examples

data(calspeedflow)
lpc1 <- lpc(calspeedflow[,3:4])
plot(lpc1, type=c("spline","project"), lwd=2)

print.lpc  Printing output for lpc and lpc.spline objects

Description

Takes an object of class lpc or lpc.spline and displays some standard output.

Usage

## S3 method for class 'lpc'
print( x, digits = max(3, getOption("digits") - 3), ...)
## S3 method for class 'lpc.spline'
print( x, digits = max(3, getOption("digits") - 3), ...)

Arguments

x  an object of class lpc or lpc.spline.
digits  not yet in use.
...  further arguments.

Value

Some short text.

Author(s)

JE

See Also

lpc

Examples

data(calspeedflow)
lpc1 <- lpc(calspeedflow[,3:4])
print(lpc1)
lpc2 <- lpc.spline(lpc1)
print(lpc2)
Measuring goodness-of-fit for principal objects.

Description

These functions compute the ‘coverage coefficient’ \( R_C \) for local principal curves, local principal points (i.e., kernel density estimates obtained through iterated mean shift), and other principal objects.

Usage

\[
\text{Rc}(x,...) \\
\text{## S3 method for class 'lpc'} \\
\text{Rc}(x,...) \\
\text{## S3 method for class 'lpc.spline'} \\
\text{Rc}(x,...) \\
\text{## S3 method for class 'ms'} \\
\text{Rc}(x,...) \\
\text{base.Rc(data, closest.coords, type="curve")}
\]

Arguments

- **x**: an object used to select a method.
- **...**: Further arguments passed to or from other methods (not needed yet).
- **data**: A data matrix.
- **closest.coords**: A matrix of coordinates of the projected data.
- **type**: For principal curves, don’t modify. For principal points, set "points".

Details

\( \text{Rc} \) computes the coverage coefficient \( R_C \), a quantity which estimates the goodness-of-fit of a fitted principal object. This quantity can be interpreted similar to the coefficient of determination in regression analysis: Values close to 1 indicate a good fit, while values close to 0 indicate a ‘bad’ fit (corresponding to linear PCA).

For objects of type \text{lpc}, \text{lpc.spline}, and \text{ms}, S3 methods are available which use the generic function \text{Rc}. This, in turn, calls the base function \text{base.Rc}, which can also be used manually if the fitted object is of another class. In principle, function \text{base.Rc} can be used for assessing goodness-of-fit of any principal object provided that the coordinates (closest.coords) of the projected data are available. For instance, for HS principal curves fitted via \text{princurve}, this information is contained in component \$s, and for a a k-means object, say \text{fitk}, this information can be obtained via \text{fitk$centers[fitk$cluster,].} Set type="points" in the latter case.

The function \text{Rc} attempts to compute all missing information, so computation will take the longer the less informative the given object \( x \) is. Note also, \text{Rc} looks up the option scaled in the fitted
object, and accounts for the scaling automatically. Important: If the data were scaled, then do NOT unscale the results by hand in order to feed the unscaled version into base.Rc, this will give a wrong result.

In terms of methodology, these functions compute $R_C$ directly through the mean reduction of absolute residual length, rather than through the area above the coverage curve.

These functions do currently not account for observation weights, i.e. $R_C$ is computed through the unweighted mean reduction in absolute residual length (even if weights have been used for the curve fitting).

Acknowledgements

Contributions (in form of pieces of code, or useful suggestions for improvements) by Jo Dwyer, Mohammad Zayed, and Ben Oakley are gratefully acknowledged.

Author(s)

J. Einbeck and L. Evers.

References


See Also

lpc.spline, codems, coverage.

Examples

data(calspeedflow)
lpc1 <- lpc.spline(lpc(calspeedflow[,3:4]), project=TRUE)
Rc(lpc1)
# is the same as:
base.Rc(lpc1$lpcobject$data, lpc1$closest.coords)

ms1 <- ms(calspeedflow[,3:4],plotms=0)
Rc(ms1)
# is the same as:
base.Rc(ms1$data, ms1$cluster.center[ms1$closest.label[, type="points"]}
Description
unscale takes an object of type lpc, lpc.spline, or ms, which had been fitted using option scaled=TRUE, and transforms the scaled components back to the original data scale.

Usage
unscale(x, ...)

## S3 method for class 'lpc'
unscale(x, ...)

## S3 method for class 'lpc.spline'
unscale(x, ...)

## S3 method for class 'ms'
unscale(x, ...)

Arguments
x an object used to select a method.
... Further arguments passed to or from other methods (not needed yet).

Value
A list of relevant items, such as LPC, start, cluster.centers, etc., which gives the unscaled versions of these quantities (some of them may carry the value NULL, if the corresponding information was not available from x).

Author(s)
JE

See Also
lpc, lpc.spline, ms

Examples
data(gvessel)
unscale(lpc(gvessel[,c(2,4,5)], h=0.11, x0=c(35, 1870, 6.3)) )
Index

*Topic datasets
  calspeedflow, 3
gaia, 8
gvessel, 10
*Topic multivariate
  coverag, 4
  lpc, 12
  lpc.project, 16
  lpc.spline, 17
  LPCM-package, 2
  ms, 20
  plot.lpc, 22
  print.lpc, 24
  Rc, 25
  unscale, 27
*Topic smooth
  lpc, 12
  lpc.spline, 17
  LPCM-package, 2
base.Rc (Rc), 25
calspeedflow, 3
coverage, 4, 26
distancevector (kernels.and.distances), 11
enorm (kernels.and.distances), 11
followx, 7
gaia, 8
gvessel, 10
dkex (kernels.and.distances), 11
kern (kernels.and.distances), 11
kernd (kernels.and.distances), 11
kernels.and.distances, 11
lpc, 2, 5–7, 12, 17, 18, 23, 24, 27
lpc.control, 5, 13, 14
lpc.coverage, 2
lpc.coverage (coverage), 4
lpc.curve.length
  (lpc.spline.auxiliary.functions), 19
lpc.fit.spline
  (lpc.spline.auxiliary.functions), 19
lpc.project, 2, 16
lpc.project.spline
  (lpc.spline.auxiliary.functions), 19
lpc.self.coverage, 2, 21
lpc.self.coverage (coverage), 4
lpc.spline, 2, 17, 17, 19, 23, 26, 27
lpc.spline.auxiliary.functions, 19
lpc.spline.eval
  (lpc.spline.auxiliary.functions), 19
lpc.splinefun
  (lpc.spline.auxiliary.functions), 19
LPCM (LPCM-package), 2
LPCM-package, 2
meanshift (ms), 20
mindist (kernels.and.distances), 11
ms, 2, 20, 26, 27
plot.lpc, 22
print.lpc, 24
Rc, 2, 21, 25
select.self.coverage (coverage), 4
unscale, 13, 27
vecdist (kernels.and.distances), 11