# Package 'fdapace'

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Type Package

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Description A versatile package that provides implementation of various methods of Functional Data Analysis (FDA) and Empirical Dynamics. The core of this package is Functional Principal Component Analysis (FPCA), a key technique for functional data analysis, for sparsely or densely sampled random trajectories and time courses, via the Principal Analysis by Conditional Estimation (PACE) algorithm. This core algorithm yields covariance and mean functions, eigenfunctions and principal component (scores), for both functional data and derivatives, for both dense (functional) and sparse (longitudinal) sampling designs. For sparse designs, it provides fitted continuous trajectories with confidence bands, even for subjects with very few longitudinal observations. PACE is a viable and flexible alternative to random effects modeling of longitudinal data. There is also a Matlab version (PACE) that contains some methods not available on fdapace and vice versa. Updates to fdapace were supported by grants from NIH Echo and NSF DMS-1712864 and DMS-2014626.

Please cite our package if you use it (You may run the command citation(``fdapace") to get the citation format and bibtex entry).

References: Wang, J.L., Chiou, J., Müller, H.G. (2016) <doi:10.1146/annurev-statistics-041715-033624>; Chen, K., Zhang, X., Petersen, A., Müller, H.G. (2017) <doi:10.1007/s12561-015-9137-5>.

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LinkingTo Rcpp, RcppEigen

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**BwNN** 

Minimum bandwidth based on kNN criterion.

## **Description**

Input a list of time points Lt, and the number of unique neighbors k. Obtain the minimum bandwidth guaranteeing k unique neighbours.

#### Usage

```
BwNN(Lt, k = 3, onlyMean = FALSE, onlyCov = FALSE)
```

#### **Arguments**

Lt n-by-1 list of vectors

k number of unique neighbors for cov and mu (default = 3)
onlyMean Indicator to return only the minimum bandwidth for the mean
onlyCov Indicator to return only the minimum bandwidth for the covariance

### **Examples**

```
tinyGrid = list(c(1,7), c(2,3), 6, c(2,4), c(4,5)) 
 BwNN(tinyGrid, k = 2) \# c(3,2)
```

CheckData

Check data format

### **Description**

Check if there are problems with the form and basic structure of the functional data 'y' and the recorded times 't'.

### Usage

```
CheckData(y, t)
```

### **Arguments**

```
y is a n-by-1 list of vectors
t is a n-by-1 list of vectors
```

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CheckOptions	Check option format

### **Description**

Check if the options structure is valid and set the NULL options

### Usage

```
CheckOptions(t, optns, n)
```

### **Arguments**

t is a n-by-1 list of vectors
optns is an initialized option list
n is a total number of sample curves

ConvertSupport Convert support of a mu/phi/cov etc. to and from obsGrid and work-Grid

# Description

Convert the support of a given function 1-D or 2-D function from fromGrid to toGrid. Both grids need to be sorted. This is an interpolation/convenience function.

### Usage

```
ConvertSupport(
  fromGrid,
  toGrid,
  mu = NULL,
  Cov = NULL,
  phi = NULL,
  isCrossCov = FALSE
)
```

## **Arguments**

fromGrid vector of points with input grid to interpolate from toGrid vector of points with the target grid to interpolate on

mu any vector of function to be interpolated

Cov a square matrix supported on fromGrid \* fromGrid, to be interpolated to toGrid

\* toGrid.

6 CreateBasis

phi any matrix, each column containing a function to be interpolated isCrossCov logical, indicating whether the input covariance is a cross-covariance. If so then the output is not made symmetric.

CreateBasis

Create an orthogonal basis of K functions in [0, 1], with nGrid points.

### **Description**

Create an orthogonal basis of K functions in [0, 1], with nGrid points.

# Usage

```
CreateBasis(
   K,
   pts = seq(0, 1, length.out = 50),
   type = c("cos", "sin", "fourier", "legendre01", "poly")
)
```

### **Arguments**

K A positive integer specifying the number of eigenfunctions to generate.

pts A vector specifying the time points to evaluate the basis functions.

type A string for the type of orthogonal basis.

#### Value

A K by nGrid matrix, each column containing an basis function.

```
basis <- CreateBasis(3, type='fourier')
head(basis)</pre>
```

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	Functional Principal plot	Component An	nalysis Bandwidth	Diagnostics
--	------------------------------	--------------	-------------------	-------------

#### **Description**

This function by default creates the mean and first principal modes of variation plots for 50 If provided with a derivative options object (?FPCAder) it will return the differentiated mean and first two principal modes of variation for 50

### Usage

```
CreateBWPlot(fpcaObj, derOptns = NULL, bwMultipliers = NULL)
```

### **Arguments**

fpca0bj An FPCA class object returned by FPCA().

derOptns A list of options to control the derivation parameters; see ?FPCAder. If NULL

standard diagnostics are returned

bwMultipliers A vector of multipliers that the original 'bwMu' and 'bwCov' will be multiplied

by. (default: c(0.50, 0.75, 1.00, 1.25, 1.50)) - default: NULL

### **Examples**

CreateCovPlot Creates a correlation surface plot based on the results from FPCA() or FPCder().

### **Description**

This function will open a new device if not instructed otherwise.

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#### Usage

```
CreateCovPlot(
  fpcaObj,
  covPlotType = "Fitted",
  corr = FALSE,
  isInteractive = FALSE,
  colSpectrum = NULL,
  ...
)
```

#### **Arguments**

fpca0bj returned object from FPCA().

covPlotType a string specifying the type of covariance surface to be plotted: 'Smoothed': plot

the smoothed cov surface 'Fitted': plot the fitted cov surface

corr a boolean value indicating whether to plot the fitted covariance or correlation

surface from the fpca object TRUE: fitted correlation surface; FALSE: fitted

covariance surface; default is FALSE; Only plotted for fitted fpca objects

isInteractive an option for interactive plot: TRUE: interactive plot; FALSE: printable plot

colSpectrum character vector to be use as input in the 'colorRampPalette' function defining

the colouring scheme (default: c('blue','red'))

... other arguments passed into persp3d, persp3D, plot3d or points3D for plotting

options

# Examples

CreateDesignPlot

Create design plots for functional data. See Yao, F., Müller, H.G., Wang, J.L. (2005). Functional data analysis for sparse longitudinal data. J. American Statistical Association 100, 577-590 for interpretation and usage of these plots. This function will open a new device as default.

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### **Description**

Create design plots for functional data. See Yao, F., Müller, H.G., Wang, J.L. (2005). Functional data analysis for sparse longitudinal data. J. American Statistical Association 100, 577-590 for interpretation and usage of these plots. This function will open a new device as default.

#### Usage

```
CreateDesignPlot(
  Lt,
  obsGrid = NULL,
  isColorPlot = TRUE,
  noDiagonal = TRUE,
  addLegend = TRUE,
  ...
)
```

### **Arguments**

a list of observed time points for functional data
obsGrid a vector of sorted observed time points. Default are the unique time points in Lt.
isColorPlot an option for colorful plot: TRUE: create color plot with color indicating counts
FALSE: create black and white plot with dots indicating observed time pairs
noDiagonal an option specifying plotting the diagonal design points: TRUE: remove diagonal time pairs FALSE: do not remove diagonal time pairs
addLegend Logical, default TRUE
Other arguments passed into plot().

#### **Examples**

```
set.seed(1)
n <- 20
pts <- seq(0, 1, by=0.05)
sampWiener <- Wiener(n, pts)
sampWiener <- Sparsify(sampWiener, pts, 10)
CreateDesignPlot(sampWiener$Lt, sort(unique(unlist(sampWiener$Lt))))</pre>
```

CreateDiagnosticsPlot Functional Principal Component Analysis Diagnostics plot

#### **Description**

Deprecated. Use plot. FPCA instead.

Plotting the results of an FPCA, including printing the design plot, mean function, scree-plot and the first three eigenfunctions for a functional sample. If provided with a derivative options object (?FPCAder), it will return the differentiated mean function and first two principal modes of variation for 50%, 75%, 100%, 125% and 150% of the defined bandwidth choice.

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### Usage

```
CreateDiagnosticsPlot(...)
## S3 method for class 'FPCA'
plot(x, openNewDev = FALSE, addLegend = TRUE, ...)
```

#### **Arguments**

... passed into plot.FPCA.

x An FPCA class object returned by FPCA().

openNewDev A logical specifying if a new device should be opened - default: FALSE

addLegend A logical specifying whether to add legend.

#### **Details**

The black, red, and green curves stand for the first, second, and third eigenfunctions, respectively. plot.FPCA is currently implemented only for the original function, but not a derivative FPCA object.

### **Examples**

CreateFuncBoxPlot Create functional boxplot using 'bagplot', 'KDE' or 'pointwise' methodology

### **Description**

Using an FPCA object create a functional box-plot based on the function scores. The green line corresponds to the functional median, the dark gray area to the area spanned by the curves within the 25th and 75-th percentile and the light gray to the area spanned by the curves within the 2.5th and 97.5-th percentile.

### Usage

```
CreateFuncBoxPlot(fpcaObj, optns = list(), ...)
```

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### Arguments

fpcaObj	An object of class FPCA returned by the function FPCA().
optns	A list of options control parameters specified by list(name=value). See 'Details'.
	Additional arguments for the 'plot' function.

#### **Details**

Available control options are

**ifactor** inflation ifactor for the bag-plot defining the loop of bag-plot or multiplying ifactor the KDE pilot bandwidth matrix. (see ?aplpack::compute.bagplot; ?ks::Hpi respectively; default: 2.58; 2 respectively).

variant string defining the method used ('KDE', 'pointwise' or 'bagplot') (default: 'bagplot')

unimodal logical specifying if the KDE estimate should be unimodal (default: FALSE, relevant only for variant='KDE')

addIndx vector of indices corresponding to which samples one should overlay (Default: NULL)

K integer number of the first K components used for the representation. (default: length(fpcaObj\$lambda ))

#### References

P. J. Rousseeuw, I. Ruts, J. W. Tukey (1999): The bagplot: a bivariate boxplot, The American Statistician, vol. 53, no. 4, 382-387

# Examples

CreateModeOfVarPlot

Functional Principal Component Analysis: Mode of variation plot

#### **Description**

Creates the k-th mode of variation plot around the mean. The red-line is the functional mean, the grey shaded areas show the range of variation around the mean:  $\pm Q\sqrt{\lambda_k}\phi_k$  for the dark grey area Q=1, and for the light grey are Q=2. In the case of 'rainbowPlot' the blue edge corresponds to Q=-3, the green edge to Q=+3 and the red-line to Q=0 (the mean).

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#### Usage

```
CreateModeOfVarPlot(
  fpcaObj,
  k = 1,
  rainbowPlot = FALSE,
  colSpectrum = NULL,
  ...
)
```

#### **Arguments**

fpca0bj An FPCA class object returned by FPCA().

k The k-th mode of variation to plot (default k = 1)

rainbowPlot Indicator to create a rainbow-plot instead of a shaded plot (default: FALSE)

colSpectrum Character vector to be use as input in the 'colorRampPalette' function defining the outliers colours (default: c("blue", "red", "green"), relevant only for rainbow-Plot=TRUE)

# **Examples**

Additional arguments for the plot function.

CreateOutliersPlot

Functional Principal Component or Functional Singular Value Decomposition Scores Plot using 'bagplot' or 'KDE' methodology

# Description

This function will create, using the first components scores, a set of convex hulls of the scores based on 'bagplot' or 'KDE' methodology.

#### Usage

```
CreateOutliersPlot(fObj, optns = NULL, ...)
```

CreateOutliersPlot 13

### Arguments

f0bj	A class object returned by FPCA() or FSVD().
------	--

optns A list of options control parameters specified by list(name=value). See 'De-

tails'.

... Additional arguments for the 'plot' function.

#### **Details**

Available control options are

**ifactor** inflation ifactor for the bag-plot defining the loop of bag-plot or multiplying ifactor the KDE pilot bandwidth matrix. (see ?aplpack::compute.bagplot; ?ks::Hpi respectively; default: 2.58; 2 respectively).

variant string defining the outlier method used ('KDE', 'NN' or 'bagplot') (default: 'KDE')

**unimodal** logical specifying if the KDE estimate should be unimodal (default: FALSE, relevant only for variant='KDE')

**maxVar** logical specifying if during slicing we should used the directions of maximum variance (default: FALSE for FPCA, TRUE for FSVD)

**nSlices** integer between 3 and 16, denoting the number of slices to be used (default: 4, relevant only for groupingType='slice')

**showSlices** logical specifying if during slicing we should show the outline of the slice (default: FALSE)

**colSpectrum** character vector to be use as input in the 'colorRampPalette' function defining the outliers colours (default: c("red", "yellow", 'blue'), relevant only for groupingType='slice')

**grouping Type** string specifying if a slice grouping ('slice') or a standard percentile/bagplot grouping ('standard') should be returned (default: 'standard')

**fIndices** a two-component vector with the index of the mode of variation to consider (default: c(1,2) for FPCA and c(1,1) for FSVD)

#### Value

An (temporarily) invisible copy of a list containing the labels associated with each of sample curves.

#### References

P. J. Rousseeuw, I. Ruts, J. W. Tukey (1999): The bagplot: a bivariate boxplot, The American Statistician, vol. 53, no. 4, 382-387 R. J. Hyndman and H. L. Shang. (2010) Rainbow plots, bagplots, and boxplots for functional data, Journal of Computational and Graphical Statistics, 19(1), 29-45

```
set.seed(1)
n <- 420
pts <- seq(0, 1, by=0.05)
sampWiener <- Wiener(n, pts)</pre>
```

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CreatePathPlot

*Create the fitted sample path plot based on the results from FPCA().* 

# Description

Create the fitted sample path plot based on the results from FPCA().

### Usage

```
CreatePathPlot(
  fpcaObj,
  subset,
  K = NULL,
  inputData = fpcaObj[["inputData"]],
  showObs = !is.null(inputData),
  obsOnly = FALSE,
  showMean = FALSE,
  derOptns = list(p = 0),
  ...
)
```

# Arguments

fpcaObj	Returned object from FPCA().
subset	A vector of indices or a logical vector for subsetting the observations.
K	The number of components to reconstruct the fitted sample paths.
inputData	A list of length 2 containing the sparse/dense (unsupported yet) observations. inputData needs to contain two fields: Lt for a list of time points and Ly for a list of observations. Default to the 'inputData' field within 'fpcaObj'.
show0bs	Whether to plot the original observations for each subject.
obs0nly	Whether to show only the original curves.
showMean	Whether to plot the mean function as a bold solid curve.
derOptns	A list of options to control derivation parameters; see 'fitted.FPCA'. (default = $NULL$ )
	other arguments passed into matplot for plotting options

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#### **Examples**

```
set.seed(1)
n <- 20
pts <- seq(0, 1, by=0.05)
sampWiener <- Wiener(n, pts)</pre>
sampWiener <- Sparsify(sampWiener, pts, 10)</pre>
res <- FPCA(sampWiener$Ly, sampWiener$Lt,</pre>
            list(dataType='Sparse', error=FALSE, kernel='epan',
            verbose=TRUE))
CreatePathPlot(res, subset=1:5)
# CreatePathPlot has a lot of usages:
CreatePathPlot(res)
CreatePathPlot(res, 1:20)
CreatePathPlot(res, 1:20, showObs=FALSE)
CreatePathPlot(res, 1:20, showMean=TRUE, showObs=FALSE)
CreatePathPlot(res, 1:20, obsOnly=TRUE)
CreatePathPlot(res, 1:20, obsOnly=TRUE, showObs=FALSE)
CreatePathPlot(inputData=sampWiener, subset=1:20, obsOnly=TRUE)
```

CreateScreePlot

Create the scree plot for the fitted eigenvalues

### **Description**

This function will open a new device if not instructed otherwise.

# Usage

```
CreateScreePlot(fpcaObj, ...)
```

### **Arguments**

```
fpca0bj A object of class FPCA returned by the function FPCA().
... Additional arguments for the 'plot' function.
```

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CreateStringingPlot

Create plots for observed and stringed high dimensional data

### Description

The function produces the following three plots: 1) A plot of predictors (standardized if specified so during stringing) in original order for a subset of observations; 2) A plot of predictors in stringed order for the same subset of observations; 3) A plot of the stringing function, which is the stringed order vs. the original order.

### Usage

```
CreateStringingPlot(stringingObj, subset, ...)
```

# **Arguments**

stringing0bj A stringing object of class "Stringing", returned by the function Stringing.

Subset A vector of indices or a logical vector for subsetting the observations. If missing, first min(n,50) observations will be plotted where n is the sample size.

Other arguments passed into matplot for plotting options

# Details

This approach is based on Chen, K., Chen, K., Müller, H.G., Wang, J.L. (2011). Stringing high-dimensional data for functional analysis. J. American Statistical Association 106, 275–284.

```
set.seed(1)
n <- 50
wiener = Wiener(n = n)[,-1]
p = ncol(wiener)
rdmorder = sample(size = p, x=1:p, replace = FALSE)
stringingfit = Stringing(X = wiener[,rdmorder], disOptns = "correlation")
diff_norev = sum(abs(rdmorder[stringingfit$StringingOrder] - 1:p))
diff_rev = sum(abs(rdmorder[stringingfit$StringingOrder] - p:1))
if(diff_rev <= diff_norev){
    stringingfit$StringingOrder = rev(stringingfit$StringingOrder)
    stringingfit$Ly = lapply(stringingfit$Ly, rev)
}
CreateStringingPlot(stringingfit, 1:20)</pre>
```

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Cumulative Trapezoid Rule Numerical Integration

### **Description**

Cumulative Trapezoid Rule Numerical Integration using Rcpp

### Usage

```
cumtrapzRcpp(X, Y)
```

#### **Arguments**

Χ	Sorted	vector	of X	values

Y Vector of Y values.

Dynamical Correlation

#### **Description**

Calculates the Dynamical Correlation for 2 paired dense regular functional data observed on the same grid.

### Usage

```
DynCorr(x, y, t)
```

### **Arguments**

X	a n by m matrix where rows representing subjects and columns representing
	measurements, missings are allowed.
V	an by m matrix where rows representing subjects and columns representing

y a n by m matrix where rows representing subjects and columns representing measurements, missings are allowed.

t a length m vector of time points where x,y are observed.

### Value

A length n vector of individual dynamic correlations. The dynamic correlation can be obtained by taking average of this vector.

#### References

Dubin J A, Müller H G. Dynamical correlation for multivariate longitudinal data (2005). Journal of the American Statistical Association 100(471): 872-881. Liu S, Zhou Y, Palumbo R, Wang, J.L. (2016). Dynamical correlation: A new method for quantifying synchrony with multivariate intensive longitudinal data. Psychological methods 21(3): 291.

Dyn\_test

#### **Examples**

```
set.seed(10)
n=200
                  # sample size
t=seq(0,1,length.out=100)
                              # length of data
mu_quad_x=8*t^2-4*t+5
mu_quad_y=8*t^2-12*t+6
fun=rbind(rep(1,length(t)),-t,t^2)
z1=matrix(0,n,3)
z1[,1]=rnorm(n,0,2)
z1[,2]=rnorm(n,0,16/3)
z1[,3]=rnorm(n,0,4)
x1\_quad\_error=y1\_quad\_error=matrix(0,nrow=n,ncol=length(t))
for (i in 1:n){
  x1_quad_error[i,]=mu_quad_x+z1[i,]%*%fun+rnorm(length(t),0,0.01)
  y1_quad_error[i,]=mu_quad_y+2*z1[i,]%*%fun +rnorm(length(t),0,0.01)
dyn1_quad=DynCorr(x1_quad_error,y1_quad_error,t)
```

Dyn\_test

Bootstrap test of Dynamic Correlation

### **Description**

Perform one sample (H0: Dynamic correlation = 0) or two sample (H0:Dynamic\_correlation\_1 = Dynamic\_correlation\_2) bootstrap test of H\_0: Dynamical Correlation=0.

### Usage

```
Dyn_{test}(x1, y1, t1, x2, y2, t2, B = 1000)
```

# **Arguments**

x1	a n by m matrix where rows representing subjects and columns representing measurements, missings are allowed.
y1	a n by m matrix where rows representing subjects and columns representing measurements, missings are allowed.
t1	a vector of time points where x1,y1 are observed.
x2	(optional if missing will be one sample test) a n by m matrix where rows representing subjects and columns representing measurements, missings are allowed.
y2	(optional if missing will be one sample test) a n by m matrix where rows representing subjects and columns representing measurements, missings are allowed.
t2	(optional if missing will be one sample test) a vector of time points where x2,y2 are observed.
В	number of bootstrap samples.

#### Value

```
a list of the following
stats Test statistics.
pval p-value of the test.
```

#### References

Dubin J A, Müller H G. (2005) Dynamical correlation for multivariate longitudinal data. Journal of the American Statistical Association 100(471): 872-881.

Liu S, Zhou Y, Palumbo R, Wang, J.L. (2016). Dynamical correlation: A new method for quantifying synchrony with multivariate intensive longitudinal data. Psychological Methods 21(3): 291.

### **Examples**

```
n=20
                 # sample size
t=seq(0,1,length.out=100)
                                # length of data
mu_quad_x=8*t^2-4*t+5
mu\_quad\_y=8*t^2-12*t+6
fun=rbind(rep(1,length(t)),-t,t^2)
z1=matrix(0,n,3)
z1[,1]=rnorm(n,0,2)
z1[,2]=rnorm(n,0,16/3)
z1[,3]=rnorm(n,0,4) # covariance matrix of random effects
x1_quad_error=y1_quad_error=matrix(0,nrow=n,ncol=length(t))
for (i in 1:n){
 x1_quad_error[i,]=mu_quad_x+z1[i,]%*%fun+rnorm(length(t),0,0.01)
 y1_quad_error[i,]=mu_quad_y+2*z1[i,]%*%fun +rnorm(length(t),0,0.01)
bt_DC=Dyn_test(x1_quad_error,y1_quad_error,t,B=500) # using B=500 for speed consideration
```

FAM

Functional Additive Models

#### **Description**

Functional additive models with a single predictor process

# Usage

```
FAM(
   Y,
   Lx,
   Lt,
   nEval = 51,
   newLx = NULL,
   newLt = NULL,
```

```
bwMethod = 0,
alpha = 0.7,
supp = c(-2, 2),
optns = NULL
```

### **Arguments**

Υ	An <i>n</i> -dimensional vector whose elements consist of scalar responses.
Lx	A list of $n$ vectors containing the observed values for each individual. See FPCA for detail.
Lt	A list of $n$ vectors containing the observation time points for each individual. Each vector should be sorted in ascending order. See FPCA for detail.
nEval	The number of evaluation grid points for kernel smoothing (default is 51. If it is specified as 0, then estimated FPC scores in the training set are used for evaluation grid instead of equal grid).
newLx	A list of the observed values for test set. See predict. FPCA for detail.
newLt	A list of the observed time points for test set. See predict.FPCA for detail.
bwMethod	The method of bandwidth selection for kernel smoothing, a positive value for designating K-fold cross-validtaion and zero for GCV (default is 50)
alpha	The shrinkage factor (positive number) for bandwidth selection. See Han et al. (2016) (default is 0.7).
supp	The lower and upper limits of kernel smoothing domain for studentized FPC scores, which FPC scores are divided by the square roots of eigenvalues (default is [-2,2]).
optns	A list of options control parameters specified by list(name=value). See FPCA.

### **Details**

FAM fits functional additive models for a scalar response and single predictor process proposed by Müller and Yao (2007) that

$$E(Y|\mathbf{X}) = \sum_{k=1}^{K} g_k(\xi_k),$$

where  $\xi_k$  stand for the k-th FPC score of the the predictor process.

### Value

A list containing the following fields:

mu	Mean estimator of $EY$
fam	A $N$ by $K$ matrix whose column vectors consist of the component function estimators at the given estimation points.
xi	An $N$ by $K$ matrix whose column vectors consist of $N$ vectors of estimation points for each component function.
bw	A K-dimensional bandwidth vector.

1 ambda A *K*-dimensional vector containing eigenvalues.

phi An *nWorkGrid* by *K* matrix containing eigenfunctions, supported by WorkGrid.

See FPCA.

workGrid An nWorkGrid by K\_j working grid, the internal regular grid on which the eigen

analysis is carried on. See FPCA.

#### References

Müller, H.-G. and Yao, F. (2005), "Functional additive models", JASA, Vol.103, No.484, p.1534-1544

```
set.seed(1000)
library(MASS)
f1 \leftarrow function(t) 0.5*t
f2 <- function(t) 2*cos(2*pi*t/4)</pre>
f3 \leftarrow function(t) 1.5*sin(2*pi*t/4)
f4 <- function(t) 2*atan(2*pi*t/4)
n <- 100
N <- 100
sig <- diag(c(4.0,2.0,1.5,1.2))
scoreX <- mvrnorm(n,mu=rep(0,4),Sigma=sig)</pre>
scoreXTest <- mvrnorm(N,mu=rep(0,4),Sigma=sig)</pre>
Y \leftarrow f1(scoreX[,1]) + f2(scoreX[,2]) + f3(scoreX[,3]) + f4(scoreX[,4]) + rnorm(n,0,0.1)
YTest <- f1(scoreXTest[,1]) + f2(scoreXTest[,2]) +
  f3(scoreXTest[,3]) + f4(scoreXTest[,4]) + rnorm(N,0,0.1)
phi1 <- function(t) sqrt(2)*sin(2*pi*t)</pre>
phi2 <- function(t) sqrt(2)*sin(4*pi*t)</pre>
phi3 <- function(t) sqrt(2)*cos(2*pi*t)</pre>
phi4 <- function(t) sqrt(2)*cos(4*pi*t)</pre>
grid <- seq(0,1,length.out=21)</pre>
Lt <- Lx <- list()
for (i in 1:n) {
  Lt[[i]] \leftarrow grid
  Lx[[i]] <- scoreX[i,1]*phi1(grid) + scoreX[i,2]*phi2(grid) +</pre>
    scoreX[i,3]*phi3(grid) + scoreX[i,4]*phi4(grid) + rnorm(1,0,0.01)
}
LtTest <- LxTest <- list()
for (i in 1:N) {
  LtTest[[i]] <- grid
  LxTest[[i]] <- scoreXTest[i,1]*phi1(grid) + scoreXTest[i,2]*phi2(grid) +</pre>
    scoreXTest[i,3]*phi3(grid) + scoreXTest[i,4]*phi4(grid) + rnorm(1,0,0.01)
```

```
}
# estimation
fit <- FAM(Y=Y,Lx=Lx,Lt=Lt)</pre>
xi <- fit$xi
op <- par(mfrow=c(2,2))</pre>
j <- 1
g1 <- f1(sort(xi[,j]))</pre>
tmpSgn <- sign(sum(g1*fit$fam[,j]))</pre>
plot(sort(xi[,j]),g1,type='l',col=2,ylim=c(-2.5,2.5),xlab='xi1')
points(sort(xi[,j]),tmpSgn*fit$fam[order(xi[,j]),j],type='l')
j <- 2
g2 <- f2(sort(xi[,j]))</pre>
tmpSgn <- sign(sum(g2*fit$fam[,j]))</pre>
plot(sort(xi[,j]),g2,type='l',col=2,ylim=c(-2.5,2.5),xlab='xi2')
points(sort(xi[,j]),tmpSgn*fit$fam[order(xi[,j]),j],type='1')
j <- 3
g3 <- f3(sort(xi[,j]))
tmpSgn <- sign(sum(g3*fit$fam[,j]))</pre>
plot(sort(xi[,j]),g3,type='1',col=2,ylim=c(-2.5,2.5),xlab='xi3')
points(sort(xi[,j]),tmpSgn*fit$fam[order(xi[,j]),j],type='1')
j <- 4
g4 <- f4(sort(xi[,j]))
tmpSgn <- sign(sum(g4*fit$fam[,j]))</pre>
plot(sort(xi[,j]),g4,type='1',col=2,ylim=c(-2.5,2.5),xlab='xi4')
points(sort(xi[,j]),tmpSgn*fit$fam[order(xi[,j]),j],type='1')
par(op)
# fitting
fit <- FAM(Y=Y,Lx=Lx,Lt=Lt,nEval=0)</pre>
yHat <- fit$mu+apply(fit$fam,1,'sum')</pre>
plot(yHat,Y)
abline(coef=c(0,1),col=2)
# R^2
R2 \leftarrow 1-sum((Y-yHat)^2)/sum((Y-mean(Y))^2)
R2
# prediction
fit <- FAM(Y=Y,Lx=Lx,Lt=Lt,newLx=LxTest,newLt=LtTest)</pre>
yHat <- fit$mu+apply(fit$fam,1,'sum')</pre>
plot(yHat,YTest,xlim=c(-10,10))
abline(coef=c(0,1),col=2)
```

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FCCor	Calculation of functional correlation between two simultaneously observed processes.
	servea processes.

# Description

Calculation of functional correlation between two simultaneously observed processes.

# Usage

```
FCCor(
    x,
    y,
    Lt,
    bw = stop("bw missing"),
    kern = "epan",
    Tout = sort(unique(unlist(Lt)))
)
```

# Arguments

x	A list of function values corresponding to the first process.
у	A list of function values corresponding to the second process.
Lt	A list of time points for both x and y.
bw	A numeric vector for bandwidth of length either 5 or 1, specifying the bandwidths for $E(X)$ , $E(Y)$ , $var(X)$ , $var(Y)$ , and $cov(X, Y)$ . If bw is a scalar then all five bandwidths are chosen to be the same.
kern	Smoothing kernel for mu and covariance; "rect", "gauss", "epan", "gausvar", "quar" (default: "gauss")
Tout	Output time points. Default to the sorted unique time points.

# **Details**

FCCor calculate only the concurrent correlation corr(X(t), Y(t)) (note that the time points t are the same). It assumes no measurement error in the observed values.

### Value

A list with the following components:

corr	A vector of the correlation $corr(X(t), Y(t))$ evaluated at Tout.
Tout	Same as the input Tout.
bw	The bandwidths used for $E(X)$ , $E(Y)$ , $var(X)$ , $var(Y)$ , and $cov(X, Y)$ .

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#### **Examples**

```
set.seed(1)
n <- 200
nGridIn <- 50
sparsity <- 1:5 # must have length > 1
bw < -0.2
kern <- 'epan'
T <- matrix(seq(0.5, 1, length.out=nGridIn))
## Corr(X(t), Y(t)) = 1/2
A <- Wiener(n, T)
B <- Wiener(n, T)
C <- Wiener(n, T) + matrix((1:nGridIn) , n, nGridIn, byrow=TRUE)</pre>
X \leftarrow A + B
Y \leftarrow A + C
indEach <- lapply(1:n, function(x) sort(sample(nGridIn, sample(sparsity, 1))))</pre>
tAll <- lapply(1:n, function(i) T[indEach[[i]]])
Xsp <- lapply(1:n, function(i) X[i, indEach[[i]]])</pre>
Ysp <- lapply(1:n, function(i) Y[i, indEach[[i]]])</pre>
plot(T, FCCor(Xsp, Ysp, tAll, bw)[['corr']], ylim=c(-1, 1))
abline(h=0.5)
```

FClust

Functional clustering and identifying substructures of longitudinal data

### Description

Default: Cluster functional data using the functional principal component (FPC) scores obtained from the data FPC analysis using EMCluster (Chen and Maitra, 2015) or directly clustering the functional data using kCFC (Chiou and Li, 2007).

#### Usage

```
FClust(Ly, Lt, k = 3, cmethod = "EMCluster", optnsFPCA = NULL, optnsCS = NULL)
```

### **Arguments**

Ly	A list of <i>n</i> vectors containing the observed values for each individual. Missing values specified by NAs are supported for dense case (dataType='dense').
Lt	A list of $n$ vectors containing the observation time points for each individual corresponding to y.
k	A scalar defining the number of clusters to define; default 3.
cmethod	A string specifying the clustering method to use ('EMCluster' or 'kCFC'); default: 'EMCluster'.

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optnsFPCA A list of options control parameters specified by list(name=value) to be used

for by FPCA on the sample y; by default: "list( methodMuCovEst ='smooth', FVEthreshold= 0.90, methodBwCov = 'GCV', methodBwMu = 'GCV')". See

'Details in ?FPCA'.

optnsCS A list of options control parameters specified by list(name=value) to be used

for cluster-specific FPCA from kCFC; by default: "list( methodMuCovEst ='smooth', FVEthreshold= 0.70, methodBwCov = 'GCV', methodBwMu = 'GCV')". See

'Details in ?FPCA' and '?kCFC'.

#### **Details**

Within EMCluster, uses the model initiated EMCluster::em.EM and returns the optimal model based on EMCluster::emcluster. See ?EMCluster::emcluster for details.

#### Value

A list containing the following fields:

cluster A vector of levels 1:k, indicating the cluster to which each curve is allocated.

fpca An FPCA object derived from the sample used by Rmixmod, otherwise NULL.

cluster0bj Either a EMCluster object or kCFC object.

#### References

Wei-Chen Chen and Ranjan Maitra, "EMCluster: EM Algorithm for Model-Based Clustering of Finite Mixture Gaussian Distribution". (2015)

Julien Jacques and Cristian Preda, "Funclust: A curves clustering method using functional random variables density approximation". Neurocomputing 112 (2013): 164-171

Jeng-Min Chiou and Pai-Ling Li, "Functional clustering and identifying substructures of longitudinal data". Journal of the Royal Statistical Society B 69 (2007): 679-699

26 FCReg

**FCReg** 

Functional Concurrent Regression using 2D smoothing

### **Description**

Functional concurrent regression with dense or sparse functional data for scalar or functional dependent variables. Note: function-to-scalar regression can also be handled using the VCAM function in fdapace.

# Usage

```
FCReg(
  vars,
  userBwMu,
  userBwCov,
  outGrid,
  kern = "gauss",
  measurementError = TRUE,
  diag1D = "none",
  useGAM = FALSE,
  returnCov = TRUE
)
```

# Arguments

vars A l	list of input functional/scalar o	covariates. Each field	corresponds to a func-
----------	-----------------------------------	------------------------	------------------------

tional (a list) or scalar (a vector) covariate. The last entry is assumed to be the response if no entry is names 'Y'. If a field corresponds to a functional covariate, it should have two fields: 'Lt', a list of time points, and 'Ly', a list of function

values.

userBwMu A scalar with bandwidth used for smoothing the mean

userBwCov A scalar with bandwidth used for smoothing the auto- and cross-covariances

outGrid A vector with the output time points

kern Smoothing kernel choice, common for mu and covariance; "rect", "gauss", "epan",

"gausvar", "quar" (default: "gauss")

measurementError

Indicator measurement errors on the functional observations should be assumed. If TRUE the diagonal raw covariance will be removed when smoothing. (de-

fault: TRUE)

diag1D A string specifying whether to use 1D smoothing for the diagonal line of the

covariance. 'none': don't use 1D smoothing; 'cross': use 1D only for cross-covariances; 'all': use 1D for both auto- and cross-covariances. (default: 'none')

useGAM Indicator to use gam smoothing instead of local-linear smoothing (semi-parametric

option) (default: FALSE)

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returnCov

Indicator to return the covariance surfaces, which is a four dimensional array. The first two dimensions correspond to outGrid and the last two correspond to the covariates and the response, i.e. (i, j, k, l) entry being  $Cov(X_k(t_i), X_l(t_j))$  (default: FALSE)

#### **Details**

If measurement error is assumed, the diagonal elements of the raw covariance will be removed. This could result in highly unstable estimate if the design is very sparse, or strong seasonality presents. WARNING! For very sparse functional data, setting measurementError = TRUE is not recommended.

#### Value

A list containing the following fields:

beta A matrix for the concurrent regression effects, where rows correspond to differ-

ent predictors and columns to different time points.

beta0 A vector containing the time-varying intercept.

outGrid A vector of the output time points.

cov A 4-dimensional array for the (cross-)covariance surfaces, with the (i, j, k, l)

entry being Cov(X\_k(t\_i), X\_l(t\_j))

R2 A vector of the time-varying R2.

n The sample size.

#### References

Yao, F., Müller, H.G., Wang, J.L. "Functional Linear Regression Analysis for Longitudinal Data." Annals of Statistics 33, (2005): 2873-2903. (Dense data) Sentürk, D., Müller, H.G. "Functional varying coefficient models for longitudinal data." J. American Statistical Association, 10, (2010): 1256–1264. Sentürk, D., Nguyen, D.V. "Varying Coefficient Models for Sparse Noise-contaminated Longitudinal Data", Statistica Sinica 21(4), (2011): 1831-1856. (Sparse data)

```
# Y(t) = \beta_0(t) + \beta_1(t) X_1(t) + \beta_2(t) Z_2 + \epsilon

# Settings
set.seed(1)
n <- 75
nGridIn <- 150
sparsity <- 5:10 # Sparse data sparsity
T <- round(seq(0, 1, length.out=nGridIn), 4) # Functional data support
bw <- 0.1
outGrid <- round(seq(min(T), 1, by=0.05), 2)

# Simulate functional data
mu <- T * 2 # mean function for X_1
sigma <- 1</pre>
```

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```
beta_0 <- 0
beta_1 <- 1
beta_2 <- 1
Z \leftarrow MASS::mvrnorm(n, rep(0, 2), diag(2))
X_1 <- Z[, 1, drop=FALSE] %*% matrix(1, 1, nGridIn) + matrix(mu, n, nGridIn, byrow=TRUE)
epsilon <- rnorm(n, sd=sigma)</pre>
Y <- matrix(NA, n, nGridIn)
for (i in seq_len(n)) {
  Y[i, ] \leftarrow beta_0 + beta_1 * X_1[i, ] + beta_2 * Z[i, 2] + epsilon[i]
# Sparsify functional data
set.seed(1)
X_1sp <- Sparsify(X_1, T, sparsity)</pre>
set.seed(1)
Ysp <- Sparsify(Y, T, sparsity)</pre>
vars <- list(X_1=X_1sp, Z_2=Z[, 2], Y=Ysp)</pre>
withError2D <- FCReg(vars, bw, bw, outGrid)
```

fdapace

fdapace: Functional Data Analysis and Empirical Dynamics

#### **Description**

fdapace is a versatile package that provides implementation of various methods of Functional Data Analysis (FDA) and Empirical Dynamics. The core of this package is Functional Principal Component Analysis (FPCA), a key technique for functional data analysis, for sparsely or densely sampled random trajectories and time courses, via the Principal Analysis by Conditional Estimation (PACE) algorithm. This core algorithm yields covariance and mean functions, eigenfunctions and principal component (scores), for both functional data and derivatives, for both dense (functional) and sparse (longitudinal) sampling designs. For sparse designs, it provides fitted continuous trajectories with confidence bands, even for subjects with very few longitudinal observations. PACE is a viable and flexible alternative to random effects modeling of longitudinal data. There is also a Matlab version (PACE) that contains some methods not available on fdapace and vice versa.

#### **Details**

Links for fdapace/PACE: Matlab version of pace at http://anson.ucdavis.edu/~mueller/data/pace.html Papers and background at http://anson.ucdavis.edu/~mueller/ and http://www.stat.ucdavis.edu/~wang/

PACE is based on the idea that observed functional data are generated by a sample of underlying (but usually not fully observed) random trajectories that are realizations of a stochastic process. It does not rely on pre-smoothing of trajectories, which is problematic if functional data are sparsely sampled.

The functional principal components can be used for further statistical analysis depending on the demands of a user, for example if one has densely sampled functional predictors and a generalized response, such as in a GLM, the predictor functions can be replaced by their first couple of

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principal component scores that will then be used as predictors; one can also easily fit polynomial functional models by using powers (usually squares) and interactions of functional principal components among the predictors for a scalar response.

fdapace is a comprehensive package that directly implements fitting of the following models:

- · functional linear regression
- · functional additive regression
- functional covariance and correlation (via dynamic correlation)
- · functional clustering
- · concurrent (varying coefficient) regression models for sparse and dense designs
- · varying coefficient additive models
- multivariate functional data analysis (normalization and functional singular component analysis)
- variance processes and volatility processes (the latter of interest in finance)
- optimal designs for longitudinal data analysis (for trajectory prediction and for functional linear regression)
- stringing, a method to convert high-dimensional data into functional data
- quantile regression, with functions as predictors

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#### References

- Wang, J.L., Chiou, J., Müller, H.G. (2016). Functional data analysis. Annual Review of Statistics and Its Application 3, 257–295;
- Chen, K., Zhang, X., Petersen, A., Müller, H.G. (2017). Quantifying infinite-dimensional data: Functional Data Analysis in action. Statistics in Biosciences 9, 582—604.

#### See Also

Useful links:

- https://github.com/functionaldata/tPACE
- Report bugs at https://github.com/functionaldata/tPACE/issues

PACKAGE

fitted.FPCA

Fitted functional data from FPCA object

# Description

Combines the zero-meaned fitted values and the interpolated mean to get the fitted values for the trajectories or the derivatives of these trajectories. Estimates are given on the work-grid, not on the observation grid. Use ConvertSupport to map the estimates to your desired domain. 100\*(1-alpha)-percentage coverage intervals, or bands, for trajectory estimates (not derivatives) are provided. For details consult the example.

### Usage

```
## S3 method for class 'FPCA'
fitted(
  object,
  K = NULL,
  derOptns = list(p = 0),
  ciOptns = list(alpha = NULL, cvgMethod = NULL),
  ...
)
```

### **Arguments**

object	A object of class FPCA returned by the function FPCA().
K	The integer number of the first K components used for the representation. (default: $length(fpcaObj\$lambda\ ))$
derOptns	A list of options to control the derivation parameters specified by list(name=value). See 'Details'. (default = NULL)
ciOptns	A list of options to control the confidence interval/band specified by list(name=value). See 'Details'. (default = NULL)
	Additional arguments

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#### **Details**

Available derivation control options are

**p** The order of the derivatives returned (default: 0, max: 2)

method The method used to produce the sample of derivatives ('FPC' (default) or 'QUO'). See Liu and Müller (2009) for more details

**bw** Bandwidth for smoothing the derivatives (default: p \* 0.10 \* S)

**kernelType** Smoothing kernel choice; same available types are FPCA(). default('epan')

Available confidence interval/band control options are

**alpha** Significant level for confidence interval/band for trajectory coverage. default=0.05 (currently only work when p=0)

**cvgMethod** Option for trajectory coverage method between 'interval' (pointwise coverage) and 'band' (simultaneous coverage). default='band'

#### Value

If alpha is NULL, p>1 or functional observations are dense, an n by length(workGrid) matrix, each row of which contains a sample. Otherwise, it returns a list which consists of the following items:

workGrid An evaluation grid for fitted values.

fitted An n by length(workGrid) matrix, each row of which contains a sample.

cvgUpper An n by length(workGrid) matrix, each row of which contains the upper alpha-

coverage limit

cvgLower An n by length(workGrid) matrix, each row of which contains the lower alpha-

coverage limit

#### References

Yao, F., Müller, H.-G. and Wang, J.-L. "Functional data analysis for sparse longitudinal data", Journal of the American Statistical Association, vol.100, No. 470 (2005): 577-590.

Liu, Bitao, and Hans-Georg Müller. "Estimating derivatives for samples of sparsely observed functions, with application to online auction dynamics." Journal of the American Statistical Association 104, no. 486 (2009): 704-717. (Sparse data FPCA)

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```
cvgUpper <- fittedY$cvgUpper
cvgLower <- fittedY$cvgLower

op <- par(mfrow=c(2,3))
ind <- sample(1:n,6)
for (i in 1:6) {
   j <- ind[i]
   plot(workGrid,cvgUpper[j,],type='l',ylim=c(min(cvgLower[j,]),max(cvgUpper[j,])),col=4,lty=2,
        xlab='t', ylab='X(t)', main=paste(j,'-th subject',sep=''))
   points(workGrid,cvgLower[j,],type='l',col=4,lty=2)
   points(res$inputData$Lt[[j]],res$inputData$Ly[[j]])
}
par(op)</pre>
```

fitted.FPCAder

Fitted functional data for derivatives from the FPCAder object

### **Description**

Combines the zero-meaned fitted values and the mean derivative to get the fitted values for the derivative trajectories. Estimates are given on the work-grid, not on the observation grid. Use ConvertSupport to map the estimates to your desired domain.

### Usage

```
## S3 method for class 'FPCAder'
fitted(object, K = NULL, ...)
```

### Arguments

object A object of class FPCA returned by the function FPCA().

K The integer number of the first K components used for the representation. (default: length(derObj\$lambda))

... Additional arguments

### Value

An n by length(workGrid) matrix, each row of which contains a sample.

### References

Liu, Bitao, and Hans-Georg Müller. "Estimating derivatives for samples of sparsely observed functions, with application to online auction dynamics." Journal of the American Statistical Association 104, no. 486 (2009): 704-717. (Sparse data FPCA)

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### **Examples**

```
set.seed(1)
n <- 20
pts <- seq(0, 1, by=0.05)
sampWiener <- Wiener(n, pts)
sampWiener <- Sparsify(sampWiener, pts, 10)</pre>
```

FLM

Functional Linear Models

# Description

Functional linear models for scalar or functional responses and scalar and/or functional predictors.

### Usage

```
FLM(Y, X, XTest = NULL, optnsListY = NULL, optnsListX = NULL, nPerm = NULL)
```

# Arguments

Υ	Either an $n$ -dimensional vector whose elements consist of scalar responses, or a list which contains functional responses in the form of a list LY and the time points LT at which they are observed (i.e., list(Ly = LY,Lt = LT)).
X	A list of either (1) lists which contains the observed functional predictors list $Lxj$ and the time points list $Ltj$ at which they are observed. It needs to be of the form $list(list(Ly = Lx1, Lt = Lxt1), list(Ly = Lx2, Lt = Lxt2),)$ ; (2) a matrix containing one or more scalar covariates; or (3) a mix of (1) and (2), in which case the scalar covariates must come after the functional ones.
XTest	A list which contains the values of functional predictors for a held-out testing set.
optnsListY	A list of options control parameters for the response specified by list(name=value). See 'Details' in FPCA.
optnsListX	Either (1) A list of options control parameters for the predictors specified by list(name=value); or (2) A list of list of options, e.g. list(list(name1=value1), list(name2=value2)). See 'Details' in FPCA.
nPerm	If this argument is specified, perform a permutation test to obtain the (global) p-value for the test of regression relationship between X and Y. Recommend to set to 1000 or larger if specified.

#### Value

A list of the following:

alpha A length-one numeric if the response Y is scalar. Or a vector of length(workGridY)

of the fitted constant alpha(t) in the linear model if Y is functional.

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).

#### References

muY

Yao, F., Müller, H.G., Wang, J.L. (2005). Functional linear regression analysis for longitudinal data. Annals of Statistics 33, 2873–2903. Hall, P., Horowitz, J.L. (2007). Methodology and convergence rates for functional linear regression. The Annals of Statistics, 35(1), 70–91.

The mean or the mean function of the response

```
set.seed(1000)
library(MASS)
### functional covariate
phi1 <- function(t,k) sqrt(2)*sin(2*pi*k*t)
phi2 <- function(t,k) sqrt(2)*cos(2*pi*k*t)
lambdaX <- c(1,0.7)
# training set</pre>
```

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```
n <- 50
Xi <- matrix(rnorm(2*n),nrow=n,ncol=2)</pre>
denseLt <- list(); denseLy <- list()</pre>
sparseLt <- list(); sparseLy <- list()</pre>
t0 <- seq(0,1,length.out=51)</pre>
for (i in 1:n) {
 denseLt[[i]] <- t0</pre>
  denseLy[[i]] \leftarrow lambdaX[1]*Xi[i,1]*phi1(t0,1) + lambdaX[2]*Xi[i,2]*phi1(t0,2)
  ind <- sort(sample(1:length(t0),3))</pre>
  sparseLt[[i]] <- t0[ind]</pre>
  sparseLy[[i]] <- denseLy[[i]][ind]</pre>
}
denseX <- list(Ly=denseLy,Lt=denseLt)</pre>
sparseX <- list(Ly=sparseLy,Lt=sparseLt)</pre>
denseX <- list(X=denseX)</pre>
sparseX <- list(X=sparseX)</pre>
# test set
N <- 30
XiTest <- matrix(rnorm(2*N),nrow=N,ncol=2)</pre>
denseLtTest <- list(); denseLyTest <- list()</pre>
sparseLtTest <- list(); sparseLyTest <- list()</pre>
t0 <- seq(0,1,length.out=51)</pre>
for (i in 1:N) {
  denseLtTest[[i]] <- t0</pre>
 denseLyTest[[i]] \leftarrow lambdaX[1]*XiTest[i,1]*phi1(t0,1) + lambdaX[2]*XiTest[i,2]*phi1(t0,2)
  ind <- sort(sample(1:length(t0),5))</pre>
  sparseLtTest[[i]] <- t0[ind]</pre>
  sparseLyTest[[i]] <- denseLyTest[[i]][ind]</pre>
}
denseXTest <- list(Ly=denseLyTest,Lt=denseLtTest)</pre>
sparseXTest <- list(Ly=sparseLyTest,Lt=sparseLtTest)</pre>
denseXTest <- list(X=denseXTest)</pre>
sparseXTest <- list(X=sparseXTest)</pre>
### scalar response
beta <- c(1, -1)
Y \leftarrow c(Xi\%*\%diag(lambdaX)\%*\%beta) + rnorm(n,0,0.5)
YTest <- c(XiTest%*%diag(lambdaX)%*%beta) + rnorm(N,0,0.5)
```

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```
## dense
denseFLM <- FLM(Y=Y,X=denseX,XTest=denseXTest,optnsListX=list(FVEthreshold=0.95))</pre>
trueBetaList <- list()</pre>
trueBetaList[[1]] <- cbind(phi1(denseFLM$workGridX[[1]],1),phi1(denseFLM$workGridX[[1]],2))%*%beta</pre>
# coefficient function estimation error (L2-norm)
plot(denseFLM$workGridX[[1]],denseFLM$betaList[[1]],type='l',xlab='t',ylab=paste('beta',1,sep=''))
points(denseFLM$workGridX[[1]],trueBetaList[[1]],type='1',col=2)
denseEstErr <-
 sqrt(trapzRcpp(denseFLM$workGridX[[1]],(denseFLM$betaList[[1]] - trueBetaList[[1]])^2))
denseEstErr
op <- par(mfrow=c(1,2))</pre>
plot(denseFLM$yHat,Y,xlab='fitted Y', ylab='observed Y')
abline(coef=c(0,1),col=8)
plot(denseFLM$yPred,YTest,xlab='predicted Y', ylab='observed Y')
abline(coef=c(0,1),col=8)
par(op)
# prediction error
densePredErr <- sqrt(mean((YTest - denseFLM$yPred)^2))</pre>
densePredErr
```

FLMCI

Confidence Intervals for Functional Linear Models.

#### **Description**

Bootstrap pointwise confidence intervals for the coefficient functions in functional linear models.

### Usage

```
FLMCI(Y, X, level = 0.95, R = 999, optnsListY = NULL, optnsListX = NULL)
```

### **Arguments**

Υ	Either an n-dimensional vector whose elements consist of scalar responses, or a list which contains functional responses in the form of a list LY and the time points LT at which they are observed (i.e., list(Ly = LY, Lt = LT)).
X	A list of lists which contains the observed functional predictors list Lxj and the time points list Ltj at which they are observed. It needs to be of the form $list(list(Ly = Lx1, Lt = Lxt1), list(Ly = Lx2, Lt = Lxt2),)$ .
level	A number taking values in [0,1] determining the confidence level. Default: 0.95.
R	An integer holding the number of bootstrap replicates. Default: 999.

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optnsListY	A list of options control parameters for the response specified by list(name=value). See 'Details' in FPCA.
optnsListX	A list of options control parameters for the predictors specified by list(name=value). See 'Details' in FPCA.

## **Details**

If measurement error is assumed, the diagonal elements of the raw covariance will be removed. This could result in highly unstable estimate if the design is very sparse, or strong seasonality presents. WARNING! For very sparse functional data, setting measurementError=TRUE is not recommended.

## Value

A list containing the following fields:

CI_alpha	CI for the intercept function — A data frame holding three variables: CI_grid — the time grid where the CIs are evaluated, CI_lower and CI_upper — the lower and upper bounds of the CIs for the intercept function on CIgrid.
CI_beta	A list containing CIs for the slope functions — the length of the list is the same as the number of covariates. Each list contains the following fields: A data frame holding three variables: $CI\_grid$ — the time grid where the CIs are evaluated, $CI\_lower$ and $CI\_upper$ — the lower and upper bounds of the CIs for the coefficient function on $CIgrid$ for $j=1,2,\ldots$
level	The confidence level of the CIs.
FOptDes	Optimal Designs for Functional and Longitudinal Data for Trajectory Recovery or Scalar Response Prediction

# Description

Optimal Designs for Functional and Longitudinal Data for Trajectory Recovery or Scalar Response Prediction

```
FOptDes(
   Ly,
   Lt,
   Resp,
   p = 3,
   optns = list(),
   isRegression = !missing(Resp),
   isSequential = FALSE,
   RidgeCand = NULL
)
```

FOptDes

A list of *n* vectors containing the observed values for each individual. Missing

A vector of positive numbers as ridge penalty candidates for regularization. The

final value is selected via cross validation. If only 1 ridge parameter is specified,

# **Arguments**Ly

A list of <i>n</i> vectors containing the observation time points for each individual corresponding to y. Each vector should be sorted in ascending order.  Resp A vector of response values, keep void for trajectory recovery, only necessary for scalar response prediction task.  p A fixed positive integer indicating the number of optimal design points requested, with default: 3.  optns A list of options control parameters specified by list(name=value) for FPCA, with default: list().  isRegression A logical argument, indicating the purpose of the optimal designs: TRUE for scalar response prediction, FALSE for trajectory recovery, with default value !missing(Resp).  isSequential A logical argument, indicating whether to use the sequential optimization procedure for faster computation, recommended for relatively large p (default: FALSE).	J	values specified by NAs are supported for dense case (dataType='dense').
for scalar response prediction task.  p	Lt	1
with default: 3.  optns A list of options control parameters specified by list(name=value) for FPCA, with default: list().  isRegression A logical argument, indicating the purpose of the optimal designs: TRUE for scalar response prediction, FALSE for trajectory recovery, with default value !missing(Resp).  isSequential A logical argument, indicating whether to use the sequential optimization proce-	Resp	
with default: list().  isRegression A logical argument, indicating the purpose of the optimal designs: TRUE for scalar response prediction, FALSE for trajectory recovery, with default value !missing(Resp).  isSequential A logical argument, indicating whether to use the sequential optimization proce-	p	
scalar response prediction, FALSE for trajectory recovery, with default value !missing(Resp).  isSequential A logical argument, indicating whether to use the sequential optimization proce-	optns	
	isRegression	scalar response prediction, FALSE for trajectory recovery, with default value
	isSequential	

#### **Details**

RidgeCand

To select a proper RidgeCand, check with the returned optimal ridge parameter. If the selected parameter is the maximum/minimum values in the candidates, it is possible that the selected one is too small/big.

#### Value

A list containing the following fields:

OptDes The vector of optimal design points of the regular time grid of the observed data.

R2 Coefficient of determination. (Check the paper for details.)

R2adj Adjusted coefficient of determination.

CV procedure is skipped.

OptRidge The selected ridge parameter.

#### References

Ji, H., Müller, H.G. (2017) "Optimal Designs for Longitudinal and Functional Data" Journal of the Royal Statistical Society: Series B 79, 859-876.

# Examples

```
set.seed(1)
n <- 50
pts <- seq(0, 1, by=0.05)
sampWiener <- Wiener(n, pts)</pre>
```

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**FPCA** 

Functional Principal Component Analysis

## Description

FPCA for dense or sparse functional data.

#### Usage

```
FPCA(Ly, Lt, optns = list())
```

## **Arguments**

Ly	A list of $n$ vectors containing the observed values for each individual. Missing values specified by NAs are supported for dense case (dataType='Dense').
Lt	A list of $n$ vectors containing the observation time points for each individual corresponding to y. Each vector should be sorted in ascending order.
optns	A list of options control parameters specified by list(name=value). See 'Details'.

#### **Details**

If the input is sparse data, make sure you check the design plot is dense and the 2D domain is well covered by support points, using plot or CreateDesignPlot. Some study design such as snippet data (where each subject is observed only on a sub-interval of the period of study) will have an ill-covered design plot, in which case the nonparametric covariance estimate will be unreliable. WARNING! Slow computation times may occur if the dataType argument is incorrect. If FPCA is taking a while, please double check that a dense design is not mistakenly coded as 'Sparse'. Applying FPCA to a mixture of very dense and sparse curves may result in computational issues.

Available control options are

userBwCov The bandwidth value for the smoothed covariance function; positive numeric - default: determine automatically based on 'methodBwCov'

methodBwCov The bandwidth choice method for the smoothed covariance function; 'GMeanAndGCV' (the geometric mean of the GCV bandwidth and the minimum bandwidth), 'CV', 'GCV' - default: 10% of the support

**userBwMu** The bandwidth value for the smoothed mean function (using 'CV' or 'GCV'); positive numeric - default: determine automatically based on 'methodBwMu'

**methodBwMu** The bandwidth choice method for the mean function; 'GMeanAndGCV' (the geometric mean of the GCV bandwidth and the minimum bandwidth),'CV','GCV' - default: 5% of the support

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**dataType** The type of design we have (usually distinguishing between sparse or dense functional data); 'Sparse', 'Dense', 'DenseWithMV', 'p»n' - default: determine automatically based on 'IsRegular'

- diagnosticsPlot Deprecated. Same as the option 'plot'
- plot Plot FPCA results (design plot, mean, scree plot and first K (<=3) eigenfunctions); logical default: FALSE
- **error** Assume measurement error in the dataset; logical default: TRUE
- fitEigenValues Whether also to obtain a regression fit of the eigenvalues default: FALSE
- **FVEthreshold** Fraction-of-Variance-Explained threshold used during the SVD of the fitted covariance function; numeric (0,1] default: 0.99
- **FVEfittedCov** Fraction-of-Variance explained by the components that are used to construct fitted-Cov; numeric (0,1] default: NULL (all components available will be used)
- **kernel** Smoothing kernel choice, common for mu and covariance; "rect", "gauss", "epan", "gausvar", "quar" default: "gauss"; dense data are assumed noise-less so no smoothing is performed.
- kFoldMuCov The number of folds to be used for mean and covariance smoothing. Default: 10
- lean If TRUE the 'inputData' field in the output list is empty. Default: FALSE
- **maxK** The maximum number of principal components to consider default: min(20, N-2,nRegGrid-2), N:# of curves, nRegGrid:# of support points in each direction of covariance surface
- **methodXi** The method to estimate the PC scores; 'CE' (Conditional Expectation), 'IN' (Numerical Integration) default: 'CE' for sparse data and dense data with missing values, 'IN' for dense data. If time points are irregular but spacing is small enough, 'IN' method is utilized by default.
- **methodMuCovEst** The method to estimate the mean and covariance in the case of dense functional data; 'cross-sectional', 'smooth' default: 'cross-sectional'
- **nRegGrid** The number of support points in each direction of covariance surface; numeric default: 51
- **numBins** The number of bins to bin the data into; positive integer > 10, default: NULL
- **methodSelectK** The method of choosing the number of principal components K; 'FVE', 'AIC', 'BIC', or a positive integer as specified number of components: default 'FVE')
- **shrink** Whether to use shrinkage method to estimate the scores in the dense case (see Yao et al 2003) default FALSE
- **outPercent** A 2-element vector in [0,1] indicating the percentages of the time range to be considered as left and right boundary regions of the time window of observation default (0,1) which corresponds to no boundary
- **methodRho** The method of regularization (add to diagonal of covariance surface) in estimating principal component scores; 'trunc': rho is truncation of sigma2, 'ridge': rho is a ridge parameter, 'vanilla': vanilla approach default "vanilla".
- **rotationCut** The 2-element vector in [0,1] indicating the percent of data truncated during sigma^2 estimation; default (0.25, 0.75))
- **useBinnedData** Should the data be binned? 'FORCE' (Enforce the # of bins), 'AUTO' (Select the # of bins automatically), 'OFF' (Do not bin) default: 'AUTO'

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useBinnedCov Whether to use the binned raw covariance for smoothing; logical - default:TRUE

usergrid Whether to use observation grid for fitting, if false will use equidistant grid. logical default:FALSE

**userCov** The user-defined smoothed covariance function; list of two elements: numerical vector 't' and matrix 'cov', 't' must cover the support defined by 'Ly' - default: NULL

**userMu** The user-defined smoothed mean function; list of two numerical vector 't' and 'mu' of equal size, 't' must cover the support defined 'Ly' - default: NULL

userSigma2 The user-defined measurement error variance. A positive scalar. If specified then the vanilla approach is used (methodRho is set to 'vanilla', unless specified otherwise). Default to 'NULL'

**userRho** The user-defined measurement truncation threshold used for the calculation of functional principal components scores. A positive scalar. Default to 'NULL'

useBW1SE Pick the largest bandwidth such that CV-error is within one Standard Error from the minimum CV-error, relevant only if methodBwMu = 'CV' and/or methodBwCov = 'CV'; logical - default: FALSE

imputeScores Whether to impute the FPC scores or not; default: 'TRUE'

verbose Display diagnostic messages; logical - default: FALSE

#### Value

bwCov

A list containing the following fields:

tion.

sigma2	Variance for measurement error.
lambda	A vector of length K containing eigenvalues.
phi	An nWorkGrid by $K$ matrix containing eigenfunctions, supported on workGrid.
xiEst	A <i>n</i> by <i>K</i> matrix containing the FPC estimates.
xiVar	A list of length $n$ , each entry containing the variance estimates for the FPC estimates.
obsGrid	The (sorted) grid points where all observation points are pooled.
mu	A vector of length nWorkGrid containing the mean function estimate.
workGrid	A vector of length nWorkGrid. The internal regular grid on which the eigen analysis is carried on.
smoothedCov	A nWorkGrid by nWorkGrid matrix of the smoothed covariance surface.
fittedCov	A nWorkGrid by nWorkGrid matrix of the fitted covariance surface, which is guaranteed to be non-negative definite.
fittedCorr	A nWorkGrid by nWorkGrid matrix of the fitted correlation surface computed from fittedCov.
optns	A list of actually used options.
timings	A vector with execution times for the basic parts of the FPCA call.
bwMu	The selected (or user specified) bandwidth for smoothing the mean function.

The selected (or user specified) bandwidth for smoothing the covariance func-

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rho A regularizing scalar for the measurement error variance estimate.

cumFVE A vector with the fraction of the cumulative total variance explained with each

additional FPC.

FVE A fraction indicating the total variance explained by chosen FPCs with corre-

sponding 'FVEthreshold'.

selectK Number *K* of selected components.

criterionValue A scalar specifying the criterion value obtained by the selected number of com-

ponents with specific methodSelectK: FVE, AIC, BIC values or NULL for fixed

K.

inputData A list containing the original 'Ly' and 'Lt' lists used as inputs to FPCA. NULL

if 'lean' was specified to be TRUE.

#### References

Yao, F., Müller, H.G., Clifford, A.J., Dueker, S.R., Follett, J., Lin, Y., Buchholz, B., Vogel, J.S. (2003). "Shrinkage estimation for functional principal component scores, with application to the population kinetics of plasma folate." Biometrics 59, 676-685. (Shrinkage estimates for dense data)

Yao, Fang, Müller, Hans-Georg and Wang, Jane-Ling (2005). "Functional data analysis for sparse longitudinal data." Journal of the American Statistical Association 100, no. 470 577-590. (Sparse data FPCA)

Liu, Bitao and Müller, Hans-Georg (2009). "Estimating derivatives for samples of sparsely observed functions, with application to online auction dynamics." Journal of the American Statistical Association 104, no. 486 704-717. (Sparse data FPCA)

Castro, P. E., Lawton, W.H. and Sylvestre, E.A. (1986). "Principal modes of variation for processes with continuous sample curves." Technometrics 28, no. 4, 329-337. (modes of variation for dense data FPCA)

## **Examples**

**FPCAder** 

Obtain the derivatives of eigenfunctions/ eigenfunctions of derivatives (note: these two are not the same)

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#### **Description**

Obtain the derivatives of eigenfunctions/ eigenfunctions of derivatives (note: these two are not the same)

#### Usage

```
FPCAder(fpcaObj, derOptns = list(p = 1))
```

## **Arguments**

fpca0bj A object of class FPCA returned by the function FPCA().

derOptns A list of options to control the derivation parameters specified by list(name=value).

See 'Details'. (default = NULL)

#### **Details**

Available derivative options are

**method** The method used for obtaining the derivatives – default is 'FPC', which is the derivatives of eigenfunctions; 'DPC': eigenfunctions of derivatives, with G^(1,1) estimated by an initial kernel local smoothing step for G^(1,0), then applying a 1D smoother in the second direction; 'FPC': functional principal component, based on smoothing the eigenfunctions; 'FPC1': functional principal component, based on smoothing G^(1,0). The latter may produce better estimates than 'FPC' but is slower.

**p** The order of the derivatives returned (default: 1, max: 2).

**bw** Bandwidth for the 1D and the 2D smoothers (default: p \* 0.1 \* S, where S is the length of the domain).

**kernelType** Smoothing kernel choice; same available types are FPCA(). default('epan')

#### References

Dai, X., Tao, W., Müller, H.G. (2018). Derivative principal components for representing the time dynamics of longitudinal and functional data. Statistica Sinica 28, 1583–1609. (DPC) Liu, Bitao, and Hans-Georg Müller. "Estimating derivatives for samples of sparsely observed functions, with application to online auction dynamics." Journal of the American Statistical Association 104, no. 486 (2009): 704-717. (FPC)

#### **Examples**

```
bw <- 0.2
kern <- 'epan'
set.seed(1)
n <- 50
M <- 30
pts <- seq(0, 1, length.out=M)
lambdaTrue <- c(1, 0.8, 0.1)^2
sigma2 <- 0.1
samp2 <- MakeGPFunctionalData(n, M, pts, K=length(lambdaTrue),</pre>
```

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```
lambda=lambdaTrue, sigma=sqrt(sigma2), basisType='legendre01')
samp2 <- c(samp2, MakeFPCAInputs(tVec=pts, yVec=samp2$Yn))</pre>
fpcaObj <- FPCA(samp2$Ly, samp2$Lt, list(methodMuCovEst='smooth',</pre>
                userBwCov=bw, userBwMu=bw, kernel=kern, error=TRUE))
CreatePathPlot(fpcaObj, showObs=FALSE)
FPCoptn <- list(bw=bw, kernelType=kern, method='FPC')</pre>
DPCoptn <- list(bw=bw, kernelType=kern, method='DPC')</pre>
FPC <- FPCAder(fpcaObj, FPCoptn)</pre>
DPC <- FPCAder(fpcaObj, DPCoptn)</pre>
CreatePathPlot(FPC, ylim=c(-5, 10))
CreatePathPlot(DPC, ylim=c(-5, 10))
# Get the true derivatives
phi <- CreateBasis(K=3, type='legendre01', pts=pts)</pre>
basisDerMat <- apply(phi, 2, function(x)
                     ConvertSupport(seq(0, 1, length.out=M - 1), pts, diff(x) * (M - 1))
trueDer <- matrix(1, n, M, byrow=TRUE) + tcrossprod(samp2$xi, basisDerMat)</pre>
matplot(t(trueDer), type='l', ylim=c(-5, 10))
# DPC is slightly better in terms of RMSE
mean((fitted(FPC) - trueDer)^2)
mean((fitted(DPC) - trueDer)^2)
```

**FPCquantile** 

Conditional Quantile estimation with functional covariates

# Description

Main function to implement conditional Quantile estimation with functional covariates and scalar response. The method includes 3 steps: 1) FPCA using the PACE method for  $X(t_x)$  2) Computation of the conditional distribution function through a functional generalized linear model. 3) Prediction of quantiles for given predictor values

```
FPCquantile(
   Lx,
   Lt_x,
   y,
   outQ = c(0.1, 0.25, 0.5, 0.75, 0.9),
   optns_x = NULL,
   isNewSub = NULL
)
```

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# Arguments

Lx	A length n list of predictor function where $x[[i]]$ is the row vector of measurements for ith subject, $i=1,,n$
Lt_x	A length n list where the observations of x are taken, $t_x[[i]]$ is a row vector of time points where $x[[i]]$ are observed, $i=1,,n$
У	A 1*n vector for scalar response y. $y[i]$ is the response value for the ith subject, $i = 1,,n$ .
outQ	A vector of desired quantile levels with default value out $Q = c(0.1, 0.25, 0.5, 0.75, 0.9)$ .
optns_x	A list of options for predictor x with control parameters specified by list(name=value) with default NA. See function FPCA for details.
isNewSub	A 1*n vector of 0s or 1s, where n is the total count of subjects. 0 denotes the corresponding subject is only used for training and 1 denotes the corresponding subject is only used for prediction. (default: 0's)

## Value

# A list of the following

pred_quantile	A matrix of n*length(outQ) where the first nn (number of 0s in isNewSub) rows containing fitted conditional quantiles of Y corresponding to the training subjects, and the last n-nn rows containing predicted conditional quantiles of Y corresponding to the subjects isNewSub ==1.	
pred_CDF	A matrix of $n*100$ . The ith row contains the fitted or predicted conditional distribution function $F(y X_i)$ , evaluated at an equally spaced grid of 100 points.	
b	A matrix of 50*(K+1) contains the coefficient functions, defined as $F(y X) = g(\sum_{\ell} k = 0)^K b_k(y) \xi_k$ , see equation (5) in the paper for details, where K is the number of components selected to expand the predictor functions X, and $\xi_k$ is the kth principal component score.	

## References

Chen, K., Müller, H.G. (2011). Conditional quantile analysis when covariates are functions, with application to growth data. J. Royal Statistical Society B 74, 67-89

# **Examples**

```
set.seed(10)

n = 200
npred = 50
m = 50
xi <- Wiener(n, 0:m/m)

x=list()
t_x=list()
y=numeric(n)
for(i in 1:n){</pre>
```

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```
t_x = c(t_x,list(0:m/m))
x = c(x,list(xi[i,]))
y[i] = 5*rnorm(1)+2*sum(xi[i,])
}

outQ = c(0.1,0.25,0.5,0.75,0.9,0.95)
isNewSub = c(rep(0,150),rep(1,50))
qtreg = FPCquantile(x, t_x, y, outQ,optns_x = NULL,isNewSub)
```

FSVD

Functional Singular Value Decomposition

# Description

FSVD for a pair of dense or sparse functional data.

## Usage

```
FSVD(
   Ly1,
   Lt1,
   Ly2,
   Lt2,
   FPCAoptns1 = NULL,
   FPCAoptns2 = NULL,
   SVDoptns = list()
)
```

# Arguments

Ly1	A list of $n$ vectors containing the observed values for each individual. Missing values specified by NAs are supported for dense case (dataType='dense').
Lt1	A list of $n$ vectors containing the observation time points for each individual corresponding to y. Each vector should be sorted in ascending order.
Ly2	A list of $n$ vectors containing the observed values for each individual. Missing values specified by NAs are supported for dense case (dataType='dense').
Lt2	A list of $n$ vectors containing the observation time points for each individual corresponding to y. Each vector should be sorted in ascending order.
FPCAoptns1	A list of options control parameters specified by list(name=value) for the FPC analysis of sample 1. See '?FPCA'.
FPCAoptns2	A list of options control parameters specified by list(name=value) for the FPC analysis of sample 2. See '?FPCA'.
SVDoptns	A list of options control parameters specified by list(name=value) for the FSVD analysis of samples 1 & 2. See 'Details'.

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#### **Details**

Available control options for SVDoptns are:

**bw1** The bandwidth value for the smoothed cross-covariance function across the direction of sample 1; positive numeric - default: determine automatically based on 'methodBwCov'

- **bw2** The bandwidth value for the smoothed cross-covariance function across the direction of sample 2; positive numeric default: determine automatically based on 'methodBwCov'
- methodBwCov The bandwidth choice method for the smoothed covariance function; 'GMeanAndGCV' (the geometric mean of the GCV bandwidth and the minimum bandwidth), 'CV', 'GCV' default: 10% of the support
- userMu1 The user defined mean of sample 1 used to centre it prior to the cross-covariance estimation. default: determine automatically based by the FPCA of sample 1
- userMu2 The user defined mean of sample 2 used to centre it prior to the cross-covariance estimation. default: determine automatically based by the FPCA of sample 2
- maxK The maximum number of singular components to consider; default: min(20, N-1), N:# of curves.
- kernel Smoothing kernel choice, common for mu and covariance; "rect", "gauss", "epan", "gausvar", "quar" default: "gauss"; dense data are assumed noise-less so no smoothing is performed.
- **rmDiag** Logical describing if the routine should remove diagonal raw cov for cross cov estimation (default: FALSE)
- **noScores** Logical describing if the routine should return functional singular scores or not (default: TRUE)
- **regulRS** String describing if the regularisation of the composite cross-covariance matrix should be done using 'sigma1' or 'rho' (see ?FPCA for details) (default: 'sigma2')
- **bwRoutine** String specifying the routine used to find the optimal bandwidth 'grid-search', 'bobyqa', 'l-bfgs-b' (default: 'l-bfgs-b')
- **flip** Logical describing if the routine should flip the sign of the singular components functions or not after the SVD of the cross-covariance matrix. (default: FALSE)
- **useGAM** Indicator to use gam smoothing instead of local-linear smoothing (semi-parametric option) (default: FALSE)
- dataType1 The type of design we have for sample 1 (usually distinguishing between sparse or dense functional data); 'Sparse', 'Dense', 'DenseWithMV' default: determine automatically based on 'IsRegular'
- **dataType2** The type of design we have for sample 2 (usually distinguishing between sparse or dense functional data); 'Sparse', 'Dense', 'DenseWithMV' default: determine automatically based on 'IsRegular'

#### Value

A list containing the following fields:

bw1 The selected (or user specified) bandwidth for smoothing the cross-covariance function across the support of sample 1.

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bw2	The selected (or user specified) bandwidth for smoothing the cross-covariance function across the support of sample 2.
CrCov	The smoothed cross-covariance between samples 1 & 2.
sValues	A list of length <i>nsvd</i> , each entry containing the singular value estimates for the FSC estimates.
nsvd	The number of singular components used.
canCorr	The canonical correlations for each dimension.
FVE	A percentage indicating the total variance explained by chosen FSCs with corresponding 'FVEthreshold'.
sFun1	An nWorkGrid by $K$ matrix containing the estimated singular functions for sample 1.
sFun2	An nWorkGrid by $K$ matrix containing the estimated singular functions for sample 2.
grid1	A vector of length nWorkGrid1. The internal regular grid on which the singular analysis is carried on the support of sample 1.
grid2	A vector of length nWorkGrid2. The internal regular grid on which the singular analysis is carried on the support of sample 2.
sScores1	A $n$ by $K$ matrix containing the singular scores for sample 1.
sScores2	A $n$ by $K$ matrix containing the singular scores for sample 2.
optns	A list of options used by the SVD and the FPCA's procedures.

# References

Yang, W., Müller, H.G., Stadtmüller, U. (2011). Functional singular component analysis. J. Royal Statistical Society B73, 303-324.

FVPA	Functional Variance Process Analysis for dense functional data

# Description

Functional Variance Process Analysis for dense functional data

```
FVPA(y, t, q = 0.1, optns = list(error = TRUE, FVEthreshold = 0.9))
```

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#### **Arguments**

У	A list of $n$ vectors containing the observed values for each individual. Missing values specified by NAs are supported for dense case (dataType='dense').
t	A list of $n$ vectors containing the observation time points for each individual corresponding to y.
q	A scalar defining the percentile of the pooled sample residual sample used for adjustment before taking log (default: 0.1).
optns	A list of options control parameters specified by list(name=value); by default: 'error' has to be TRUE, 'FVEthreshold' is set to 0.90. See 'Details in 'FPCA'.

#### Value

A list containing the following fields:

sigma2 Variance estimator of the functional variance process.

fpca0bjY FPCA object for the original data.

fpca0bjR FPCA object for the functional variance process associated with the original

data.

#### References

Hans-Georg Müller, Ulrich Stadtmüller and Fang Yao, "Functional variance processes." Journal of the American Statistical Association 101 (2006): 1007-1018

## **Examples**

```
set.seed(1)
n <- 25
pts <- seq(0, 1, by=0.01)
sampWiener <- Wiener(n, pts)
# Data have to dense for FVPA to be relevant!
sampWiener <- Sparsify(sampWiener, pts, 101)
fvpaObj <- FVPA(sampWiener$Ly, sampWiener$Lt)</pre>
```

GetCovSurface

Covariance Surface

## **Description**

Covariance surface estimation for dense or sparse functional data.

```
GetCovSurface(Ly, Lt, optns = list())
```

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#### **Arguments**

Ly

A list of n vectors containing the observed values for each individual. Missing values specified by NAs are supported for dense case (dataType='Dense').

Lt

A list of *n* vectors containing the observation time points for each individual corresponding to y. Each vector should be sorted in ascending order.

optns

A list of options control parameters specified by list(name=value). See 'Details'.

Available control options are

- **userBwCov** The bandwidth value for the smoothed covariance function; positive numeric default: determine automatically based on 'methodBwCov'
- **methodBwCov** The bandwidth choice method for the smoothed covariance function; 'GMeanAndGCV' (the geometric mean of the GCV bandwidth and the minimum bandwidth),'CV','GCV' default: 10% of the support
- userBwMu The bandwidth value for the smoothed mean function (using 'CV' or 'GCV'); positive numeric default: determine automatically based on 'methodBwMu'
- methodBwMu The bandwidth choice method for the mean function; 'GMeanAndGCV' (the geometric mean of the GCV bandwidth and the minimum bandwidth),'CV','GCV' default: 5% of the support
- **dataType** The type of design we have (usually distinguishing between sparse or dense functional data); 'Sparse', 'Dense', 'DenseWithMV', 'p»n' default: determine automatically based on 'IsRegular'
- error Assume measurement error in the dataset; logical default: TRUE
- **kernel** Smoothing kernel choice, common for mu and covariance; "rect", "gauss", "epan", "gausvar", "quar" default: "gauss"; dense data are assumed noiseless so no smoothing is performed.
- **kFoldMuCov** The number of folds to be used for mean and covariance smoothing. Default: 10
- **lean** If TRUE the 'inputData' field in the output list is empty. Default: FALSE **methodMuCovEst** The method to estimate the mean and covariance in the case of dense functional data; 'cross-sectional', 'smooth' default: 'cross-sectional'
- **nRegGrid** The number of support points in each direction of covariance surface; numeric default: 51
- **numBins** The number of bins to bin the data into; positive integer > 10, default: NULL
- **rotationCut** The 2-element vector in [0,1] indicating the percent of data truncated during sigma^2 estimation; default (0.25, 0.75))
- useBinnedData Should the data be binned? 'FORCE' (Enforce the # of bins),
   'AUTO' (Select the # of bins automatically), 'OFF' (Do not bin) default:
   'AUTO'
- useBinnedCov Whether to use the binned raw covariance for smoothing; logical default:TRUE
- userMu The user-defined smoothed mean function; list of two numerical vector 't' and 'mu' of equal size, 't' must cover the support defined 'Ly' - default: NULL

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userSigma2 The user-defined measurement error variance. A positive scalar. If specified then no regularization is used (rho is set to 'no', unless specified otherwise). Default to 'NULL'

**useBW1SE** Pick the largest bandwidth such that CV-error is within one Standard Error from the minimum CV-error, relevant only if methodBwMu = 'CV' and/or methodBwCov = 'CV'; logical - default: FALSE

#### Value

A list containing the following fields:

cov A square matrix of size nWorkGrid containing the covariance surface estimate.

sigma2 A numeric estimate of the variance of measurement error.

workGrid A vector of length nWorkGrid. The internal regular grid on which the covariance

surface estimation is carried out.

bwCov The selected (or user specified) bandwidth for smoothing the covariance surface.

A list of actually-used options relevant to the covariance surface calculation.

## **Examples**

```
set.seed(1)
n <- 20
pts <- seq(0, 1, by=0.025)
sampWiener <- Wiener(n, pts)
mu = sin(2*pi*pts)
sampWiener <- Sparsify(t(t(sampWiener) + mu), pts, 10)
res = GetCovSurface(Ly = sampWiener$Ly, Lt = sampWiener$Lt)</pre>
```

GetCrCorYX

Create cross-correlation matrix from auto- and cross-covariance ma-

trix

# Description

Create cross-correlation matrix from auto- and cross-covariance matrix

## Usage

```
GetCrCorYX(ccXY, ccXX, ccYY)
```

# Arguments

ccXY	The cross-covariance matrix between variables X and Y.
ccXX	The auto-covariance matrix of variable X or the diagonal of that matrix.
ccYY	The auto-covariance matrix of variable Y or the diagonal of that matrix.

## Value

A cross-correlation matrix between variables X and Y.

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GetCrCorYZ	Create cross-correlation matrix from auto- and cross-covariance matrix

# Description

Create cross-correlation matrix from auto- and cross-covariance matrix

## Usage

```
GetCrCorYZ(ccYZ, acYY, covZ)
```

# Arguments

ccYZ	The cross-covariance vector between variables Y and Z (n-by-1).
acYY	The auto-covariance n-by-n matrix of variable Y or the (n-by-1) diagonal of that matrix.
covZ	The (scalar) covariance of variable Z.

#### Value

A cross-correlation matrix between variables Y (functional) and Z (scalar).

GetCrCovYX	Functional Cross Covariance between longitudinal variable Y and
	longitudinal variable X

# Description

Calculate the raw and the smoothed cross-covariance between functional predictors using bandwidth bw or estimate that bw using GCV.

```
GetCrCovYX(
  bw1 = NULL,
  bw2 = NULL,
  Ly1,
  Lt1 = NULL,
  Ymu1 = NULL,
  Ly2,
  Lt2 = NULL,
  Ymu2 = NULL,
  useGAM = FALSE,
  rmDiag = FALSE,
```

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```
kern = "gauss",
bwRoutine = "l-bfgs-b"
)
```

# Arguments

bw1	Scalar bandwidth for smoothing the cross-covariance function (if NULL it will be automatically estimated) $(Y)$
bw2	Scalar bandwidth for smoothing the cross-covariance function (if NULL it will be automatically estimated) $(X)$
Ly1	List of N vectors with amplitude information (Y)
Lt1	List of N vectors with timing information (Y)
Ymu1	Vector Q-1 Vector of length nObsGrid containing the mean function estimate $(Y)$
Ly2	List of N vectors with amplitude information (X)
Lt2	List of N vectors with timing information (X)
Ymu2	Vector Q-1 Vector of length nObsGrid containing the mean function estimate $(X)$
useGAM	Indicator to use gam smoothing instead of local-linear smoothing (semi-parametric option) (default: FALSE)
rmDiag	Indicator to remove the diagonal element when smoothing (default: FALSE)
kern	String specifying the kernel type (default: FALSE; see ?FPCA for details)
bwRoutine	String specifying the routine used to find the optimal bandwidth 'grid-search', 'bobyqa', 'l-bfgs-b' (default: 'l-bfgs-b') If the variables Ly1 and Ly2 are in matrix form the data are assumed dense and only the raw cross-covariance is returned. One can obtain Ymu1 and Ymu2 from FPCA and ConvertSupport.

## Value

## A list containing:

smoothedCC The smoothed cross-covariance as a matrix (currently only 51 by 51)

rawCC The raw cross-covariance as a list

bw The bandwidth used for smoothing as a vector of length 2

score The GCV score associated with the scalar used

smoothGrid The grid over which the smoothed cross-covariance is evaluated

## References

Yang, Wenjing, Hans-Georg Müller, and Ulrich Stadtmüller. "Functional singular component analysis." Journal of the Royal Statistical Society: Series B (Statistical Methodology) 73.3 (2011): 303-324

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## **Examples**

```
Ly1= list( rep(2.1,7), rep(2.1,3),2.1 );
Lt1 = list(1:7,1:3, 1);
Ly2 = list( rep(1.1,7), rep(1.1,3),1.1);
Lt2 = list(1:7,1:3, 1);
Ymu1 = rep(55,7);
Ymu2 = rep(1.1,7);
AA<-GetCrCovYX(Ly1 = Ly1, Ly2= Ly2, Lt1=Lt1, Lt2=Lt2, Ymu1=Ymu1, Ymu2=Ymu2)</pre>
```

GetCrCovYZ

Functional Cross Covariance between longitudinal variable Y and scalar variable Z

## **Description**

Calculate the raw and the smoothed cross-covariance between functional and scalar predictors using bandwidth bw or estimate that bw using GCV

## Usage

```
GetCrCovYZ(
  bw = NULL,
  Z,
  Zmu = NULL,
  Ly,
  Lt = NULL,
  Ymu = NULL,
  support = NULL,
  kern = "gauss"
)
```

# Arguments

bw	Scalar bandwidth for smoothing the cross-covariance function (if NULL it will be automatically estimated)
Z	Vector N-1 Vector of length N with the scalar function values
Zmu	Scalar with the mean of Z (if NULL it will be automatically estimated)
Ly	List of N vectors with amplitude information
Lt	List of N vectors with timing information
Ymu	Vector Q-1 Vector of length nObsGrid containing the mean function estimate
support	Vector of unique and sorted values for the support of the smoothed cross-covariance function (if NULL it will be automatically estimated)
kern	Kernel type to be used. See ?FPCA for more details. (default: 'gauss') If the variables Ly1 is in matrix form the data are assumed dense and only the raw cross-covariance is returned. One can obtain Ymu1 from FPCA and ConvertSupport.

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## Value

## A list containing:

smoothedCC The smoothed cross-covariance as a vector rawCC The raw cross-covariance as a vector

bw The bandwidth used for smoothing as a scalar score The GCV score associated with the scalar used

#### References

Yang, Wenjing, Hans-Georg Müller, and Ulrich Stadtmüller. "Functional singular component analysis." Journal of the Royal Statistical Society: Series B (Statistical Methodology) 73.3 (2011): 303-324

# **Examples**

```
Ly <- list( runif(5), c(1:3), c(2:4), c(4))

Lt <- list( c(1:5), c(1:3), c(1:3), 4)

Z = rep(4,4) # Constant vector so the covariance has to be zero.

sccObj = GetCrCovYZ(bw=1, Z= Z, Ly=Ly, Lt=Lt, Ymu=rep(4,5))
```

GetMeanCI Bootstrap pointwise confidence intervals for the mean function for densely observed data.

## **Description**

Note that bootstrap pointwise confidence intervals do not work for sparsely observed data.

## Usage

```
GetMeanCI(Ly, Lt, level = 0.95, R = 999, optns = list())
```

# Arguments

Ly	A list of n vectors containing the observed values for each individual. Missing values specified by NAs are supported for dense case (dataType='dense').
Lt	A list of n vectors containing the observation time points for each individual corresponding to each element in Ly. Each vector should be sorted in ascending order.
level	A number taking values in [0,1] determing the confidence level. Default: 0.95.
R	An integer holding the number of bootstrap replicates. Default: 999.
optns	A list of options; see FPCA for details.

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#### Value

A list of two elements:

CI A data frame holding three variables: CIgrid — the time grid where the CIs

are evaluated; lower and upper — the lower and upper bounds of the CIs on

CIgrid.

level The confidence level of the CIs

.

## **Examples**

```
n <- 30
tgrid <- seq(0,1,length.out=21)
phi1 <- function(t) sqrt(2)*sin(2*pi*t)
phi2 <- function(t) sqrt(2)*sin(4*pi*t)
Lt <- rep(list(tgrid), n)
Ly <- lapply(1:n, function(i){
  tgrid + rnorm(1,0,2) * phi1(tgrid) + rnorm(1,0,0.5) * phi2(tgrid) + rnorm(1,0,0.01)
  })
res <- GetMeanCI(Lt = Lt, Ly = Ly, level = 0.9)</pre>
```

GetMeanCurve

Mean Curve

# Description

Mean curve calculation for dense or sparse functional data.

#### Usage

```
GetMeanCurve(Ly, Lt, optns = list())
```

# Arguments

Ly A list of n vectors containing the observed values for each individual. Missing

values specified by NAs are supported for dense case (dataType='Dense').

Lt A list of *n* vectors containing the observation time points for each individual

corresponding to y. Each vector should be sorted in ascending order.

optns A list of options control parameters specified by list(name=value). See 'De-

tails'.

Available control options are

userBwMu The bandwidth value for the smoothed mean function (using 'CV' or 'GCV'); positive numeric - default: determine automatically based on 'methodBwMu'

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methodBwMu The bandwidth choice method for the mean function; 'GMeanAndGCV' (the geometric mean of the GCV bandwidth and the minimum bandwidth),'CV','GCV' - default: 5% of the support

**dataType** The type of design we have (usually distinguishing between sparse or dense functional data); 'Sparse', 'Dense', 'DenseWithMV', 'p»n' - default: determine automatically based on 'IsRegular'

plot Plot mean curve; logical - default: FALSE

**kernel** Smoothing kernel choice, common for mu and covariance; "rect", "gauss", "epan", "gausvar", "quar" - default: "gauss"; dense data are assumed noiseless so no smoothing is performed.

**kFoldMuCov** The number of folds to be used for mean and covariance smoothing. Default: 10

**methodMuCovEst** The method to estimate the mean and covariance in the case of dense functional data; 'cross-sectional', 'smooth' - default: 'cross-sectional'

**numBins** The number of bins to bin the data into; positive integer > 10, default:

useBinnedData Should the data be binned? 'FORCE' (Enforce the # of bins),
 'AUTO' (Select the # of bins automatically), 'OFF' (Do not bin) - default:
 'AUTO'

userMu The user-defined smoothed mean function; list of two numerical vector 't' and 'mu' of equal size, 't' must cover the support defined 'Ly' - default: NULL

**useBW1SE** Pick the largest bandwidth such that CV-error is within one Standard Error from the minimum CV-error, relevant only if methodBwMu = 'CV' and/or methodBwCov = 'CV'; logical - default: FALSE

#### Value

A list containing the following fields:

mu A vector of length nWorkGrid containing the mean function estimate.

workGrid A vector of length nWorkGrid. The internal regular grid on which the mean

estimation is carried out.

bwMu The selected (or user specified) bandwidth for smoothing the mean function.

optns A list of actually-used options relevant to the mean function calculation.

#### **Examples**

```
set.seed(1)
n <- 20
pts <- seq(0, 1, by=0.025)
sampWiener <- Wiener(n, pts)
mu = sin(2*pi*pts)
sampWiener <- Sparsify(t(t(sampWiener) + mu), pts, 10)
res = GetMeanCurve(Ly = sampWiener$Ly, Lt = sampWiener$Lt, optns = list(plot = TRUE))</pre>
```

GetNormalisedSample

Normalise sparse multivariate functional data

#### **Description**

Normalise sparse functional sample given in an FPCA object

## Usage

```
GetNormalisedSample(fpcaObj, errorSigma = FALSE)
GetNormalizedSample(...)
```

## **Arguments**

fpca0bj An FPCA object.

errorSigma Indicator to use sigma^2 error variance when normalising the data (default:

FALSE)

... Passed into GetNormalisedSample

#### Value

A list containing the normalised sample 'y' at times 't'

## References

Chiou, Jeng-Min and Chen, Yu-Ting and Yang, Ya-Fang. "Multivariate Functional Principal Component Analysis: A Normalization Approach" Statistica Sinica 24 (2014): 1571-1596

## **Examples**

```
set.seed(1)
n <- 100
M <- 51
pts <- seq(0, 1, length.out=M)
mu <- rep(0, length(pts))
sampDense <- MakeGPFunctionalData(n, M, mu, K=1, basisType='sin', sigma=0.01)
samp4 <- MakeFPCAInputs(tVec=sampDense$pts, yVec=sampDense$Yn)
res4E <- FPCA(samp4$Ly, samp4$Lt, list(error=TRUE))
sampN <- GetNormalisedSample(res4E, errorSigma=TRUE)

CreatePathPlot(subset=1:20, inputData=samp4, obsOnly=TRUE, showObs=FALSE)
CreatePathPlot(subset=1:20, inputData=sampN, obsOnly=TRUE, showObs=FALSE)</pre>
```

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kCFC	Functional clustering and identifying substructures of longitudinal data using kCFC.

# Description

Functional clustering and identifying substructures of longitudinal data using kCFC.

# Usage

```
kCFC(
   y,
   t,
   k = 3,
   kSeed = 123,
   maxIter = 125,
   optnsSW = list(methodMuCovEst = "smooth", FVEthreshold = 0.9, methodBwCov = "GCV",
        methodBwMu = "GCV"),
   optnsCS = list(methodMuCovEst = "smooth", FVEthreshold = 0.7, methodBwCov = "GCV",
        methodBwMu = "GCV")
)
```

# Arguments

У	A list of $n$ vectors containing the observed values for each individual. Missing values specified by NAs are supported for dense case (dataType='dense').
t	A list of $n$ vectors containing the observation time points for each individual corresponding to y.
k	A scalar defining the number of clusters to define; default 3. Values that define very small clusters (eg.cluster size <=3) will potentially err.
kSeed	A scalar valid seed number to ensure replication; default: 123
maxIter	A scalar defining the maximum number of iterations allowed; default 20, common for both the simple kmeans initially and the subsequent k-centres
optnsSW	A list of options control parameters specified by list(name=value) to be used for sample-wide FPCA; by default: "list(methodMuCovEst='smooth', FVEthreshold= 0.90, methodBwCov = 'GCV', methodBwMu = 'GCV')". See 'Details in 'FPCA'.
optnsCS	A list of options control parameters specified by list(name=value) to be used for cluster-specific FPCA; by default: "list(methodMuCovEst='smooth', FVEthreshold= 0.70, methodBwCov = 'GCV', methodBwMu = 'GCV')". See 'Details in 'FPCA'.

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#### Value

A list containing the following fields:

cluster A vector of levels 1:k, indicating the cluster to which each curve is allocated.

fpcaList A list with the fpcaObj for each separate cluster.

iterToConv A number indicating how many iterations where required until convergence.

#### References

Jeng-Min Chiou, Pai-Ling Li, "Functional clustering and identifying substructures of longitudinal data." Journal of the Royal Statistical Society 69 (2007): 679-699

## **Examples**

Lwls1D

One dimensional local linear kernel smoother

## **Description**

One dimensional local linear kernel smoother for longitudinal data.

## Usage

```
Lwls1D(
  bw,
  kernel_type,
  win = rep(1L, length(xin)),
  xin,
  yin,
  xout,
  npoly = 1L,
  nder = 0L
)
```

#### **Arguments**

bw Scalar holding the bandwidth

kernel\_type Character holding the kernel type (see ?FPCA for supported kernels)

win Vector of length N with weights

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xin	Vector of length N with measurement points
yin	Vector of length N with measurement values
xout	Vector of length M with output measurement points
npoly	Scalar (integer) degree of polynomial fitted (default 1)
nder	Scalar (integer) degree of derivative fitted (default 0)

## Value

Vector of length M with measurement values at the the point specified by 'xout'

Lwls2D	Two dimensional local linear kernel smoother.
LWISZD	Two aimensional local linear kernel smoother.

# Description

Two dimensional local weighted least squares smoother. Only local linear smoother for estimating the original curve is available (no higher order, no derivative).

# Usage

```
Lwls2D(
  bw,
  kern = "epan",
  xin,
  yin,
  win = NULL,
  xout1 = NULL,
  xout2 = NULL,
  xout = NULL,
  xout = NULL,
  subset = NULL,
  crosscov = FALSE,
  method = ifelse(kern == "gauss", "plain", "sort2")
)
```

# Arguments

bw	A scalar or a vector of length 2 specifying the bandwidth.
kern	Kernel used: 'gauss', 'rect', 'gausvar', 'epan' (default), 'quar'.
xin	An n by 2 data frame or matrix of x-coordinate.
yin	A vector of y-coordinate.
win	A vector of weights on the observations.
xout1	a p1-vector of first output coordinate grid. Defaults to the input gridpoints if left unspecified.
xout2	a p2-vector of second output coordinate grid. Defaults to the input gridpoints if left unspecified.

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xout	alternative to xout1 and xout2. A matrix of p by 2 specifying the output points (may be inefficient if the size of xout is small).
subset	a vector with the indices of x-/y-/w-in to be used (Default: NULL)
crosscov	using function for cross-covariance estimation (Default: FALSE). FALSE for auto-covariance estimation and TRUE for two-dimensional local linear kernel smoothing or cross-covariance estimation. For auto-covariance estimation (i.e., when crosscov is FALSE), xout1 and xout2 should be the same.
method	should one try to sort the values xin and yin before using the lwls smoother? if yes ('sort2' - default for non-Gaussian kernels), if no ('plain' - fully stable; de)

## Value

a p1 by p2 matrix of fitted values if xout is not specified. Otherwise a vector of length p corresponding to the rows of xout.

Lwls2DDeriv

Two dimensional local linear kernel smoother to target derivatives.

# Description

Two dimensional local weighted least squares smoother. Only a local linear smoother for estimating the original curve is available (no higher order)

```
Lwls2DDeriv(
  bw,
  kern = "epan",
  xin,
  yin,
  win = NULL,
  xout1 = NULL,
  xout2 = NULL,
  xout = NULL,
  npoly = 1L,
  nder1 = 0L,
  nder2 = 0L,
  subset = NULL,
  crosscov = TRUE,
  method = "sort2"
)
```

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## **Arguments**

bw	A scalar or a vector of length 2 specifying the bandwidth.
kern	Kernel used: 'gauss', 'rect', 'gausvar', 'epan' (default), 'quar'.
xin	An n by 2 data frame or matrix of x-coordinate.
yin	A vector of y-coordinate.
win	A vector of weights on the observations.
xout1	a p1-vector of first output coordinate grid. Defaults to the input gridpoints if left unspecified.
xout2	a p2-vector of second output coordinate grid. Defaults to the input gridpoints if left unspecified.
xout	alternative to xout1 and xout2. A matrix of p by 2 specifying the output points (may be inefficient if the size of xout is small).
npoly	The degree of polynomials (include all $x^ay^b$ terms where $a+b \le npoly$ )
nder1	Order of derivative in the first direction
nder2	Order of derivative in the second direction
subset	a vector with the indices of x-/y-/w-in to be used (Default: NULL)
crosscov	using function for cross-covariance estimation (Default: TRUE)
method	should one try to sort the values xin and yin before using the lwls smoother? if yes ('sort2' - default for non-Gaussian kernels), if no ('plain' - fully stable; de)

#### Value

a p1 by p2 matrix of fitted values if xout is not specified. Otherwise a vector of length p corresponding to the rows of xout.

MakeBWtoZscore02y

Z-score body-weight for age 0 to 24 months based on WHO standards

# Description

Make vector of age and body-weight to z-scores based on WHO standards using LMS

# Usage

MakeBWtoZscore02y(sex, age, bw)

# Arguments

sex A character 'M' or 'F' indicating the sex of the child.

age A vector of time points of size Q.

bw A vector of body-weight readings of size Q.

## Value

A vector of Z-scores of size Q.

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MakeFPCAInputs	Format FPCA input
----------------	-------------------

# Description

Turn vector inputs to the list so they can be used in FPCA

# Usage

```
MakeFPCAInputs(
   IDs = NULL,
   tVec,
   yVec,
   na.rm = FALSE,
   sort = FALSE,
   deduplicate = FALSE)
```

# Arguments

IDs	np-by-1 vector of subject IDs (Default: NULL)
tVec	Either an np-by-1 vector of measurement times, or a p-by-1 vector corresponding to the common time support
yVec	n-by-1 vector of measurements from the variable of interest, or a n-by-p matrix with each row corresponding to the dense observations.
na.rm	logical indicating if NA should be omitted (Default: FALSE)
sort	logical indicating if Lt (and the correspoding Ly values) should be ensured to be sorted (Default: FALSE)
deduplicate	logical indicating if the Lt should be ensured not to have within-subject duplicated values; the Ly values of repeated Lt values are averaged (Default: FALSE)

# Value

L list containing 3 lists each of length 'm', 'm' being the number of unique subject IDs

# Description

For a Gaussian process, create a dense functional data sample of size n over a [0,1] support.

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#### Usage

```
MakeGPFunctionalData(
    n,
    M = 100,
    mu = rep(0, M),
    K = 2,
    lambda = rep(1, K),
    sigma = 0,
    basisType = "cos"
)
```

#### Arguments

n number of samples to generate

M number of equidistant readings per sample (default: 100)
mu vector of size M specifying the mean (default: rep(0,M))
K scalar specifying the number of basis to be used (default: 2)

lambda vector of size K specifying the variance of each components (default: rep(1,K)) sigma

The standard deviation of the Gaussian noise added to each observation points.

basisType string specifying the basis type used; possible options are: 'sin', 'cos' and 'cos' and

'fourier' (default: 'cos') (See code of 'CreateBasis' for implementation details.)

#### Value

A list containing the following fields:

Y A vector of noiseless observations.

Yn A vector of noisy observations if sigma > 0.

MakeHCtoZscore02y Z-score head-circumference for age 0 to 24 months based on WHO standards

## **Description**

Convert vector of age and height measurement to z-scores based on WHO standards using mu and sigma (not LMS)

#### **Usage**

```
MakeHCtoZscore02y(sex, age, hc)
```

# Arguments

sex A character 'M' or 'F' indicating the sex of the child.

age A vector of time points of size Q.

hc A vector of head circumference readings of size Q (in cm).

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#### Value

A vector of Z-scores of size Q.

MakeLNtoZscore02y

Z-score height for age 0 to 24 months based on WHO standards

## Description

Convert vector of age and height measurement to z-scores based on WHO standards using mu and sigma (not LMS)

## Usage

```
MakeLNtoZscore02y(sex, age, ln)
```

## Arguments

sex A character 'M' or 'F' indicating the sex of the child.

age A vector of time points of size Q.

In A vector of body-length readings of size Q (in cm).

#### Value

A vector of Z-scores of size Q.

MakeSparseGP

Create a sparse Functional Data sample for a Gaussian Process

# Description

Functional data sample of size n, sparsely sampled from a Gaussian process

```
MakeSparseGP(
    n,
    rdist = runif,
    sparsity = 2:9,
    muFun = function(x) rep(0, length(x)),
    K = 2,
    lambda = rep(1, K),
    sigma = 0,
    basisType = "cos",
    CovFun = NULL
)
```

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#### **Arguments**

n number of samples to generate.

rdist a sampler for generating the random design time points within [0, 1].

sparsity A vector of integers. The number of observation per sample is chosen to be one

of the elements in sparsity with equal chance.

muFun a function that takes a vector input and output a vector of the corresponding

mean (default: zero function).

K scalar specifying the number of basis to be used (default: 2).

lambda vector of size K specifying the variance of each components (default: rep(1,K)). sigma

The standard deviation of the Gaussian noise added to each observation points. string specifying the basis type used; possible options are: 'sin', 'cos' and

'fourier' (default: 'cos') (See code of 'CreateBasis' for implementation details.)

CovFun an alternative specification of the covariance structure.

#### Value

**TODO** 

medfly25 Number of eggs laid daily from medflies

#### **Description**

A dataset containing the eggs laid from 789 medflies (Mediterranean fruit flies, Ceratitis capitata) during the first 25 days of their lives. This is a subset of the dataset used by Carey at al. (1998); only flies that lived at least 25 days are included, i.e, at the end of the recording period [0,25] all flies are still alive.

#### Format

A data frame with 19725 rows and 3 variables:

**ID**: Medfly ID according to the original dataset

Days: Day of measurement

**nEggs**: Number of eggs laid at that particular day **nEggsRemain**: Remaining total number of eggs laid

#### Source

https://anson.ucdavis.edu/~mueller/data/medfly1000.html

#### References

Carey, J.R., Liedo, P., Müller, H.G., Wang, J.L., Chiou, J.M. (1998). Relationship of age patterns of fecundity to mortality, longevity, and lifetime reproduction in a large cohort of Mediterranean fruit fly females. J. of Gerontology –Biological Sciences 53, 245-251.

MultiFAM

Functional Additive Models with Multiple Predictor Processes

# Description

Smooth backfitting procedure for functional additive models with multiple predictor processes

# Usage

```
MultiFAM(
   Y,
   X,
   ker = "epan",
   nEval = 51,
   XTest = NULL,
   bwMethod = 0,
   alpha = 0.7,
   supp = c(-2, 2),
   optnsList = NULL
)
```

# Arguments

Υ	An <i>n</i> -dimensional vector whose elements consist of scalar responses.
X	A <i>d</i> -dimensional list whose components consist of two lists of <i>Ly</i> and <i>Lt</i> containing observation times and functional covariate values for each predictor component, respectively. For details of <i>Ly</i> and <i>Lt</i> , see FPCA for detail.
ker	A function object representing the base kernel to be used in the smooth back-fitting algorithm (default is 'epan' which is the only option supported currently).
nEval	The number of evaluation grid points for kernel smoothing (default is 51. If it is specified as 0, then estimated FPC scores in the training set are used for evaluation grid instead of equal grid).
XTest	A <i>d</i> -dimensional list for test set of functional predictors (default is NULL). If XTest is specified, then estimated FPC scores in the test set are used for evaluation grid.
bwMethod	The method of initial bandwidth selection for kernel smoothing, a positive value for designating K-fold cross-validtaion and zero for GCV (default is 0)
alpha	The shrinkage factor (positive number) for bandwidth selection. See Han et al. (2016) (default is 0.7).
supp	The lower and upper limits of kernel smoothing domain for studentized FPC scores, which FPC scores are divided by the square roots of eigenvalues (default is [-2,2]).
optnsList	A <i>d</i> -dimensional list whose components consist of optns for each predictor component, respectively. (default is NULL which assigns the same default optns for all components as in FPCA).

#### **Details**

MultiFAM fits functional additive models for a scalar response and multiple predictor processes and implements the smooth backfitting algorithm provided in Han, K., Müller, H.G., Park, B.U. (2018). Smooth backfitting for additive modeling with small errors-in-variables, with an application to additive functional regression for multiple predictor functions. Bernoulli 24, 1233–1265.

It is based on the model

$$E(Y|\mathbf{X}) = \sum_{j=1}^{d} \sum_{k=1}^{K_j} g_{jk}(\xi_{jk}),$$

where  $\xi_{jk}$  stand for the k-th FPC scores of the j-th predictor process. MultiFAM only is for the multiple predictor processes case. For a univariate predictor use FAM, the functional additive model (Müller and Yao 2008). It is necessary to designate an estimation support for the additive component functions where the additive modeling is only allowed over restricted intervals (see Han et al., 2018).

#### Value

A list containing the following fields:

mu	A scalar for the centered regression model.
SBFit	An $N$ by $(K_1 + + K_d)$ matrix whose column vectors consist of the smooth backfitting component function estimators at the given $N$ estimation points.
xi	An N by $(K_1 + + K_d)$ matrix whose column vectors consist of the FPC score grid vectors at which each additive component function is evaluated.
bw	A $(K_1 + + K_d)$ -dimensional bandwidth vector.
lambda	A $(K_1 + + K_d)$ -dimensional vector containing eigenvalues.
phi	A $d$ -dimensional list whose components consist of an $nWorkGrid$ by $K\_j$ matrix containing eigenfunctions, supported by WorkGrid. See FPCA.
workGrid	A $d$ -dimensional list whose components consist of an $nWorkGrid$ by $K\_j$ working grid, a regular grid on which the eigenanalysis is carried out See FPCA.

## References

Mammen, E., Linton, O. and Nielsen, J. (1999), "The existence and asymptotic properties of a backfitting projection algorithm under weak conditions", Annals of Statistics, Vol.27, No.5, p.1443-1490.

Mammen, E. and Park, B. U. (2006), "A simple smooth backfitting method for additive models", Annals of Statistics, Vol.34, No.5, p.2252-2271.

Müller, H.-G. and Yao, F. (2008), "Functional additive models", Journal of the American Statistical Association, Vol.103, No.484, p.1534-1544.

Han, K., Müller, H.-G. and Park, B. U. (2016), "Smooth backfitting for additive modeling with small errors-in-variables, with an application to additive functional regression for multiple predictor functions", Bernoulli (accepted).

#### **Examples**

```
set.seed(1000)
library(MASS)
f11 \leftarrow function(t) t
f12 \leftarrow function(t) 2*cos(2*pi*t/4)
f21 <- function(t) 1.5*sin(2*pi*t/4)
f22 \leftarrow function(t) 1.5*atan(2*pi*t/4)
n<-100
N<-200
sig <- matrix(c(2.0, 0.0, 0.5, -.2,
                 0.0, 1.2, -.2, 0.3,
                 0.5, -.2, 1.7, 0.0,
                 -.2, 0.3, 0.0, 1.0),
               nrow=4,ncol=4)
scoreX <- mvrnorm(n,mu=rep(0,4),Sigma=sig)</pre>
scoreXTest <- mvrnorm(N,mu=rep(0,4),Sigma=sig)</pre>
Y \leftarrow f11(scoreX[,1]) + f12(scoreX[,2]) + f21(scoreX[,3]) + f22(scoreX[,4]) + rnorm(n,0,0.5)
YTest <- f11(scoreXTest[,1]) + f12(scoreXTest[,2]) +
f21(scoreXTest[,3]) + f22(scoreXTest[,4]) + rnorm(N,0,0.5)
phi11 <- function(t) sqrt(2)*sin(2*pi*t)</pre>
phi12 <- function(t) sqrt(2)*sin(4*pi*t)</pre>
phi21 <- function(t) sqrt(2)*cos(2*pi*t)</pre>
phi22 <- function(t) sqrt(2)*cos(4*pi*t)</pre>
grid <- seq(0,1,length.out=21)</pre>
Lt <- Lx1 <- Lx2 <- list()
for (i in 1:n) {
  Lt[[i]] <- grid
  Lx1[[i]] \leftarrow scoreX[i,1]*phi11(grid) + scoreX[i,2]*phi12(grid) + rnorm(1,0,0.01)
 Lx2[[i]] <- scoreX[i,3]*phi21(grid) + scoreX[i,4]*phi22(grid) + rnorm(1,0,0.01)
}
LtTest <- Lx1Test <- Lx2Test <- list()
for (i in 1:N) {
  LtTest[[i]] <- grid</pre>
 Lx1Test[[i]] <- scoreXTest[i,1]*phi11(grid) + scoreXTest[i,2]*phi12(grid) + rnorm(1,0,0.01)</pre>
 Lx2Test[[i]] <- scoreXTest[i,3]*phi21(grid) + scoreXTest[i,4]*phi22(grid) + rnorm(1,0,0.01)</pre>
X1 <- list(Ly=Lx1, Lt=Lt)</pre>
X2 <- list(Ly=Lx2, Lt=Lt)</pre>
X1Test <- list(Ly=Lx1Test, Lt=LtTest)</pre>
X2Test <- list(Ly=Lx2Test, Lt=LtTest)</pre>
```

```
X <- list(X1, X2)</pre>
XTest <- list(X1Test, X2Test)</pre>
# estimation
sbf <- MultiFAM(Y=Y,X=X)</pre>
xi <- sbf$xi
par(mfrow=c(2,2))
j <- 1
p0 <- trapzRcpp(sort(xi[,j]),dnorm(sort(xi[,j]),0,sqrt(sig[j,j])))</pre>
g11 <- f11(sort(xi[,j])) -
trapzRcpp(sort(xi[,j]),f11(sort(xi[,j]))*dnorm(sort(xi[,j]),0,sqrt(sig[j,j])))/p0
tmpSgn <- sign(sum(g11*sbf$SBFit[,j]))</pre>
plot(sort(xi[,j]),g11,type='l',col=2,ylim=c(-2.5,2.5),xlab='xi11')
points(sort(xi[,j]),tmpSgn*sbf$SBFit[order(xi[,j]),j],type='l')
legend('top',c('true','SBF'),col=c(2,1),lwd=2,bty='n',horiz=TRUE)
j <- 2
p0 <- trapzRcpp(sort(xi[,j]),dnorm(sort(xi[,j]),0,sqrt(sig[j,j])))</pre>
g12 <- f12(sort(xi[,j])) -
trapzRcpp(sort(xi[,j]),f12(sort(xi[,j]))*dnorm(sort(xi[,j]),\emptyset,sqrt(sig[j,j])))/p\emptyset
tmpSgn <- sign(sum(g12*sbf$SBFit[,j]))</pre>
plot(sort(xi[,j]),g12,type='l',col=2,ylim=c(-2.5,2.5),xlab='xi12')
points(sort(xi[,j]),tmpSgn*sbf$SBFit[order(xi[,j]),j],type='1')
legend('top',c('true','SBF'),col=c(2,1),lwd=2,bty='n',horiz=TRUE)
j <- 3
p0 <- trapzRcpp(sort(xi[,j]),dnorm(sort(xi[,j]),0,sqrt(sig[j,j])))</pre>
g21 <- f21(sort(xi[,j])) -
trapzRcpp(sort(xi[,j]),f21(sort(xi[,j]))*dnorm(sort(xi[,j]),0,sqrt(sig[j,j])))/p0
tmpSgn <- sign(sum(g21*sbf$SBFit[,j]))</pre>
plot(sort(xi[,j]),g21,type='l',col=2,ylim=c(-2.5,2.5),xlab='xi21')
points(sort(xi[,j]),tmpSgn*sbf$SBFit[order(xi[,j]),j],type='l')
legend('top',c('true','SBF'),col=c(2,1),lwd=2,bty='n',horiz=TRUE)
j <- 4
p0 <- trapzRcpp(sort(xi[,j]),dnorm(sort(xi[,j]),0,sqrt(sig[j,j])))</pre>
g22 \leftarrow f22(sort(xi[,j])) -
trapzRcpp(sort(xi[,j]),f22(sort(xi[,j]))*dnorm(sort(xi[,j]),0,sqrt(sig[j,j])))/p0
tmpSgn <- sign(sum(g22*sbf$SBFit[,j]))</pre>
plot(sort(xi[,j]),g22,type='l',col=2,ylim=c(-2.5,2.5),xlab='xi22')
points(sort(xi[,j]),tmpSgn*sbf$SBFit[order(xi[,j]),j],type='l')
legend('top',c('true','SBF'),col=c(2,1),lwd=2,bty='n',horiz=TRUE)
# fitting
sbf <- MultiFAM(Y=Y,X=X,nEval=0)</pre>
yHat <- sbf$mu+apply(sbf$SBFit,1,'sum')</pre>
plot(yHat,Y)
abline(coef=c(0,1),col=2)
```

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```
# R^2
R2 <- 1-sum((Y-yHat)^2)/sum((Y-mean(Y))^2)
R2

# prediction
sbf <- MultiFAM(Y=Y,X=X,XTest=XTest)
yHat <- sbf$mu+apply(sbf$SBFit,1,'sum')
plot(yHat,YTest)
abline(coef=c(0,1),col=2)</pre>
```

NormCurvToArea

Normalize a curve to a particular area, by multiplication with a factor

## **Description**

Normalize a curve such that its integration over the design time-points equals a particular value (according to trapezoid integration).

#### Usage

```
NormCurvToArea(y, x = seq(0, 1, length.out = length(y)), area = 1)
```

## **Arguments**

```
y values of curve at time-points x

x design time-points (default: seq(0,1, length.out=length(y)))

area value to normalize the curve onto (default: 1)
```

## Value

values of curve at times x such that its integration over x equals area.

```
predict.FPCA Predict FPC scores and curves for a new sample given an FPCA object
```

## Description

Return a list containing the matrix with the first k FPC scores according to conditional expectation or numerical integration, the matrix of predicted trajectories and the prediction work grid.

```
## S3 method for class 'FPCA'
predict(object, newLy, newLt, sigma2 = NULL, K = NULL, xiMethod = "CE", ...)
```

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### **Arguments**

object	An FPCA object.
newLy	A list of $n$ vectors containing the observed values for each individual.
newLt	A list of $n$ vectors containing the observation time points for each individual corresponding to y.
sigma2	The user-defined measurement error variance. A positive scalar. (default: rho if applicable, otherwise sigma 2 if applicable, otherwise 0 if no error. )
К	The scalar defining the number of clusters to define; (default: from user-specified FPCA Object).
xiMethod	The integration method used to calculate the functional principal component scores (standard numerical integration 'IN' or conditional expectation 'CE'); default: 'CE'.
	Not used.

### Value

A list containing the following fields:

scores A matrix of size *n*-by-*k* which comprise of the predicted functional principal

component scores.

predCurves A matrix of size *n*-by-*l* where *l* is the length of the work grid in *object*.

predGrid A vector of length l which is the output grid of the predicted curves. This is

same is the workgrid of object.

```
set.seed(1)
n <- 50
pts <- seq(0, 1, by=0.05)
# The first n samples are for training and the rest testing
sampWiener <- Wiener(2 * n, pts)
sparsity <- 2:5
train <- Sparsify(sampWiener[seq_len(n), , drop=FALSE], pts, sparsity)
test <- Sparsify(sampWiener[seq(n + 1, 2 * n), , drop=FALSE], pts, sparsity)
res <- FPCA(train$Ly, train$Lt)
pred <- predict(res, test$Ly, test$Lt, K=3)
plot(pred$predGrid, pred$predCurves[1,])</pre>
```

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print.FPCA

Print an FPCA object

# Description

Print a simple description of an FPCA object

# Usage

```
## S3 method for class 'FPCA'
print(x, ...)
```

# Arguments

x An FPCA object.... Not used.

# **Examples**

```
set.seed(1)
n <- 20
pts <- seq(0, 1, by=0.05)
sampWiener <- Wiener(n, pts)
sampWiener <- Sparsify(sampWiener, pts, 10)
res <- FPCA(sampWiener$Ly, sampWiener$Lt)
res</pre>
```

print.FSVD

Print an FSVD object

### **Description**

Print a simple description of an FSVD object

# Usage

```
## S3 method for class 'FSVD'
print(x, ...)
```

### **Arguments**

x An FSVD object.

... Not used.

print.WFDA 75

Print a WFDA object

# Description

Print a simple description of a WFDA object

### Usage

```
## S3 method for class 'WFDA'
print(x, ...)
```

# Arguments

x A WFDA object.

... Not used.

SBFitting

Iterative Smooth Backfitting Algorithm

# Description

Smooth backfitting procedure for nonparametric additive models

# Usage

```
SBFitting(Y, x, X, h = NULL, K = "epan", supp = NULL)
```

# Arguments

Υ	An <i>n</i> -dimensional vector whose elements consist of scalar responses.
X	An $N$ by $d$ matrix whose column vectors consist of $N$ vectors of estimation points for each component function.
Χ	An $n$ by $d$ matrix whose row vectors consist of multivariate predictors.
h	A $d$ vector of bandwidths for kernel smoothing to estimate each component function.
K	A function object representing the kernel to be used in the smooth backfitting (default is 'epan', the the Epanechnikov kernel.).
supp	A $d$ by 2 matrix whose row vectors consist of the lower and upper limits of estimation intervals for each component function (default is the $d$ -dimensional unit rectangle of $[0,1]$ ).

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#### **Details**

SBFitting fits component functions of additive models for a scalar response and a multivariate predictor based on the smooth backfitting algorithm proposed by Mammen et al. (1999), see also Mammen and Park (2006), Yu et al. (2008), Lee et al. (2010, 2012) and others. SBFitting only focuses on the locally constant smooth backfitting estimator for the multivariate predictor case. Note that the fitting in the special case of a univariate predictor is the same as that provided by a local constant kernel regression estimator (Nadaraya-Watson estimator). The local polynomial approach can be extended similarly (currently omitted). Support of the multivariate predictor is assumed to be a product of closed intervals. Users should designate an estimation support for the additive component function where modeling is restricted to subintervals of the domain (see Han et al., 2016). If one puts X in the argument for the estimation points x, SBFitting returns the estimated values of the conditional mean responses given the observed predictors.

#### Value

A list containing the following fields:

SBFit An N by d matrix whose column vectors consist of the smooth backfitting com-

ponent function estimators at the given estimation points.

mY A scalar of centered part of the regression model.

NW An N by d matrix whose column vectors consist of the Nadaraya-Watson marginal

regression function estimators for each predictor component at the given estima-

tion points.

mgnDens An N by d matrix whose column vectors consist of the marginal kernel density

estimators for each predictor component at the given estimation points.

jntDens An N by N by d by d array representing the 2-dimensional joint kernel density

estimators for all pairs of predictor components at the given estimation grid. For example, [,,j,k] of the object provides the 2-dimensional joint kernel density estimator of the (j,k)-component of predictor components at the corresponding

*N* by *N* matrix of estimation grid.

itemNum The iteration number that the smooth backfitting algorithm has stopped.

itemErr The iteration error of the smooth backfitting algorithm that represents the maxi-

mum L2 distance among component functions in the last successive updates.

#### References

Mammen, E., Linton, O. and Nielsen, J. (1999), "The existence and asymptotic properties of a backfitting projection algorithm under weak conditions", Annals of Statistics, Vol.27, No.5, p.1443-1490.

Mammen, E. and Park, B. U. (2006), "A simple smooth backfitting method for additive models", Annals of Statistics, Vol.34, No.5, p.2252-2271.

Yu, K., Park, B. U. and Mammen, E. (2008), "Smooth backfitting in generalized additive models", Annals of Statistics, Vol.36, No.1, p.228-260.

Lee, Y. K., Mammen, E. and Park., B. U. (2010), "backfitting and smooth backfitting for additive quantile models", Vol.38, No.5, p.2857-2883.

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Lee, Y. K., Mammen, E. and Park., B. U. (2012), "Flexible generalized varying coefficient regression models", Annals of Statistics, Vol.40, No.3, p.1906-1933.

Han, K., Müller, H.-G. and Park, B. U. (2016), "Smooth backfitting for additive modeling with small errors-in-variables, with an application to additive functional regression for multiple predictor functions", Bernoulli (accepted).

```
set.seed(100)
n <- 100
d <- 2
X \leftarrow pnorm(matrix(rnorm(n*d),nrow=n,ncol=d)%*matrix(c(1,0.6,0.6,1),nrow=2,ncol=2))
f1 <- function(t) 2*(t-0.5)
f2 <- function(t) sin(2*pi*t)</pre>
Y \leftarrow f1(X[,1])+f2(X[,2])+rnorm(n,0,0.1)
# component function estimation
N <- 101
x <- matrix(rep(seq(0,1,length.out=N),d),nrow=N,ncol=d)</pre>
h <- c(0.12, 0.08)
sbfEst <- SBFitting(Y,x,X,h)</pre>
fFit <- sbfEst$SBFit
op <- par(mfrow=c(1,2))</pre>
plot(x[,1],f1(x[,1]),type='l',lwd=2,col=2,lty=4,xlab='X1',ylab='Y')
points(x[,1],fFit[,1],type='l',lwd=2,col=1)
points(X[,1],Y,cex=0.3,col=8)
legend('topleft',legend=c('SBF','true'),col=c(1,2),lwd=2,lty=c(1,4),horiz=FALSE,bty='n')
abline(h=0,col=8)
plot(x[,2],f2(x[,2]),type='1',lwd=2,col=2,lty=4,xlab='X2',ylab='Y')
points(x[,2],fFit[,2],type='l',lwd=2,col=1)
points(X[,2],Y,cex=0.3,col=8)
legend('topright',legend=c('SBF','true'),col=c(1,2),lwd=2,lty=c(1,4),horiz=FALSE,bty='n')
abline(h=0,col=8)
par(op)
# prediction
x <- X
h < -c(0.12, 0.08)
sbfPred <- SBFitting(Y,X,X,h)</pre>
fPred <- sbfPred$mY+apply(sbfPred$SBFit,1,'sum')</pre>
op \leftarrow par(mfrow=c(1,1))
plot(fPred,Y,cex=0.5,xlab='SBFitted values',ylab='Y')
abline(coef=c(0,1),col=8)
par(op)
```

78 SetOptions

SelectK	Selects number of functional principal components for given FPCA output and selection criteria

# Description

Selects number of functional principal components for given FPCA output and selection criteria

# Usage

```
SelectK(fpcaObj, criterion = "FVE", FVEthreshold = 0.95, Ly = NULL, Lt = NULL)
```

# Arguments

fpcaObj	A list containing FPCA related objects returned by MakeFPCAResults().
criterion	A string or positive integer specifying selection criterion for the number of functional principal components. Available options: 'FVE', 'AIC', 'BIC', or the specified number of components - default: 'FVE' For explanations of these criteria, see Yao et al (2005, JASA)
FVEthreshold	A threshold fraction to be specified by the user when using "FVE" as selection criterion: $(0,1]$ - default: NULL
Ly	A list of $n$ vectors containing the observed values for each individual - default: NULL
Lt	A list of <i>n</i> vectors containing the observation time points for each individual corresponding to Ly - default: NULL

# Value

A list including the following two fields:

K	An integer indicating the selected number of components based on given criterion.
criterion	The calculated criterion value for the selected number of components, i.e. FVE, AIC or BIC value, NULL for fixedK criterion.

# Description

Set the PCA option list

# Usage

```
SetOptions(y, t, optns)
```

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### **Arguments**

У	A list of <i>n</i> vectors	containing the ol	bserved values	for each individual.

t A list of *n* vectors containing the observation time points for each individual

corresponding to y.

optns A list of options control parameters specified by list(name=value). See 'De-

tails'.

See '?FPCA for more details. Casual users are not advised to tamper with this

function.

Sparsify	Sparsify densely observed functional data	

# Description

Given a matrix of densely observed functional data, create a sparsified sample for experimental purposes

### Usage

```
Sparsify(samp, pts, sparsity, aggressive = FALSE, fragment = FALSE)
```

### **Arguments**

samp	A matrix of dense	ly observed functional data	<ol> <li>with each row con</li> </ol>	taining one

sample.

pts A vector of grid points corresponding to the columns of samp.

sparsity A vector of integers. The number of observation per sample is chosen to be one

of the elements in sparsity with equal chance.

aggressive Sparsify in an "aggressive" manner making sure that near-by readings are ex-

cluded.

fragment Sparsify the observations into fragments, which are (almost) uniformly dis-

tributed in the time domain. Default to FALSE as not fragmenting. Otherwise a

positive number specifying the approximate length of each fragment.

### Value

A list of length 2, containing the following fields:

Lt A list of observation time points for each sample.

Ly A list of values for each sample, corresponding to the time points.

Stringing Stringing

str.FPCA

Compactly display the structure of an FPCA object

### Description

Compactly display the structure of an FPCA object

# Usage

```
## S3 method for class 'FPCA'
str(object, ...)
```

### **Arguments**

object An FPCA object
... Not used

Stringing

Stringing for High-Dimensional data

### **Description**

Converting high-dimensional data to functional data

### Usage

```
Stringing(
   X,
   Y = NULL,
   standardize = FALSE,
   disOptns = "euclidean",
   disMat = NA
)
```

### **Arguments**

Χ	A	A matrix (1	ı by p	) of data	, where	X[i,]	is the row	vector of	f measurements	for th	ne
---	---	-------------	--------	-----------	---------	-------	------------	-----------	----------------	--------	----

ith subject.

Y A vector (n by 1), where Y[i] is the response associated with X[i,]

standardize A logical variable indicating whether standardization of the input data matrix is

required, with default: FALSE.

disOptns A distance metric to be used, one of the following: "euclidean" (default), "max-

imum", "manhattan", "canberra", "binary", "minkowski", "correlation", "spearman", "hamming", "xycor", or "user". If specified as "xycor", the absolute difference of correlation between predictor and response is used. If specified as

"user", a dissimilarity matrix for the argument disMat must be provided.

disMat A user-specified dissimilarity matrix, only necessary when disOptns is "user".

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#### Value

A list containing the following fields:

Ly A list of n vectors, which are the random trajectories for all subjects identified

by the Stringing method.

Lt A list of n time points vectors, at which corresponding measurements Ly are

taken.

StringingOrder A vector representing the order of the stringing, s.t. using as column index on X

yields recovery of the underlying process.

Xin A matrix, corresponding to the input data matrix.

Xstd A matrix, corresponding to the standardized input data matrix. It is NULL if

standardize is FALSE.

#### References

Chen, K., Chen, K., Müller, H. G., and Wang, J. L. (2011). "Stringing high-dimensional data for functional analysis." Journal of the American Statistical Association, 106(493), 275-284.

### **Examples**

```
set.seed(1)
n <- 50
wiener = Wiener(n = n)[,-1]
p = ncol(wiener)
rdmorder = sample(size = p, x=1:p, replace = FALSE)
stringingfit = Stringing(X = wiener[,rdmorder], disOptns = "correlation")
diff_norev = sum(abs(rdmorder[stringingfit$StringingOrder] - 1:p))
diff_rev = sum(abs(rdmorder[stringingfit$StringedOrder] - p:1))
if(diff_rev <= diff_norev){
    stringingfit$StringingOrder = rev(stringingfit$StringingOrder)
    stringingfit$Ly = lapply(stringingfit$Ly, rev)
}
plot(1:p, rdmorder[stringingfit$StringingOrder], pch=18); abline(a=0,b=1)</pre>
```

trapzRcpp

Trapezoid Rule Numerical Integration

### **Description**

Trapezoid Rule Numerical Integration using Rcpp

### Usage

```
trapzRcpp(X, Y)
```

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# Arguments

Χ	Sorted vector of X values
Υ	Vector of Y values.

 $\mathsf{TVAM}$ 

Iterative Smooth Backfitting Algorithm

# Description

Smooth backfitting procedure for time-varying additive models

# Usage

```
TVAM(
Lt,
Ly,
LLx,
gridT = NULL,
x = NULL,
ht = NULL,
k = NULL,
x = NULL,
```

# Arguments

Lt	An $n$ -dimensional list of $N_i$ -dimensional vector whose elements consist of longitudinal time points for each $i$ -th subject.
Ly	An $n$ -dimensional list of $N_i$ -dimensional vector whose elements consist of longitudinal response observations of each $i$ -subject corresponding to $Lt$ .
LLx	A tuple of $d$ -lists, where each list represents longitudinal covariate observations of the $j$ -th component corresponding to $Lt$ and $Ly$ .
gridT	An <i>M</i> -dimensional sequence of evaluation time points for additive surface estimators. (Must be sorted in increasing orders.)
X	An $N$ by $d$ matrix whose column vectors consist of $N$ vectors of evaluation points for additive surface component estimators at each covariate value.
ht	A bandwidth for kernel smoothing in time component.
hx	A $d$ vector of bandwidths for kernel smoothing covariate components, respectively.
K	A function object representing the kernel to be used in the smooth backfitting (default is 'epan', the the Epanechnikov kernel.).

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suppT	A 2-dimensional vector consists of the lower and upper limits of estimation intervals for time component (default is $[0,1]$ ).
suppX	A $d$ by 2 matrix whose row vectors consist of the lower and upper limits of estimation intervals for each component function (default is the $d$ -dimensional unit rectangle of $[0,1]$ ).

#### **Details**

TVAM estimates component surfaces of time-varying additive models for longitudinal observations based on the smooth backfitting algorithm proposed by Zhang et al. (2013). TVAM only focuses on the local constant smooth backfitting in contrast to the original development as in Zhang et al. (2013). However, the local polynomial version can be extended similarly, so that those are omitted in the development. Especially in this development, one can designate an estimation support of additive surfaces when the additive modeling is only allowed over restricted intervals or one is interested in the modeling over the support (see Han et al., 2016).

#### Value

A list containing the following fields:

tvamComp A tuple of d-lists, where each list is given by M by N matrix whose elements

represents the smooth backfitting surface estimator of the j-component evaluated

at gridT and the j-th column of x.

tvamMean An M-dimensional vector whose elements consist of the marginal time regres-

sion function estimated at gridT.

### References

Zhang, X., Park, B. U. and Wang, J.-L. (2013), "Time-varying additive models for longitudinal data", Journal of the American Statistical Association, Vol.108, No.503, p.983-998.

Han, K., Müller, H.-G. and Park, B. U. (2018), "Smooth backfitting for additive modeling with small errors-in-variables, with an application to additive functional regression for multiple predictor functions", Bernoulli, Vol.24, No.2, p.1233-1265.

```
set.seed(1000)

n <- 30
Lt <- list()
Ly <- list()
Lx1 <- list()
Lx2 <- list()

for (i in 1:n) {
   Ni <- sample(10:15,1)

Lt[[i]] <- sort(runif(Ni,0,1))
Lx1[[i]] <- runif(Ni,0,1)
Lx2[[i]] <- runif(Ni,0,1)</pre>
```

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```
Ly[[i]] <- Lt[[i]]*(cos(2*pi*Lx1[[i]]) + sin(2*pi*Lx2[[i]])) + rnorm(Ni,0,0.1)
}
LLx <- list(Lx1,Lx2)
gridT <- seq(0,1,length.out=31)</pre>
x0 <- seq(0,1,length.out=31)</pre>
x \leftarrow cbind(x0,x0)
ht <- 0.1
hx <- c(0.1, 0.1)
tvam <- TVAM(Lt,Ly,LLx,gridT=gridT,x=x,ht=ht,hx=hx,K='epan')</pre>
g0Sbf <- tvam$tvamMean</pre>
gjSbf <- tvam$tvamComp</pre>
op <- par(mfrow=c(1,2), mar=c(1,1,1,1)+0.1)
persp(gridT,x0,gjSbf[[1]],theta=60,phi=30,
      xlab='time',ylab='x1',zlab='g1(t, x1)')
persp(gridT,x0,gjSbf[[2]],theta=60,phi=30,
      xlab='time',ylab='x2',zlab='g1(t, x2)')
par(op)
```

VCAM

Sieve estimation: B-spline based estimation procedure for timevarying additive models. The VCAM function can be used to perform function-to-scalar regression.

### **Description**

Sieve estimation: B-spline based estimation procedure for time-varying additive models. The VCAM function can be used to perform function-to-scalar regression.

# Usage

```
VCAM(Lt, Ly, X, optnAdd = list(), optnVc = list())
```

# Arguments

Lt	An $n$ -dimensional list of $N_i$ -dimensional vectors whose elements consist of longitudinal time points for each $i$ -th subject.
Ly	An $n$ -dimensional list of $N_i$ -dimensional vectors whose elements consist of longitudinal response observations of each $i$ -subject corresponding to $Lt$ .
X	An <i>n</i> by <i>d</i> matrix whose row vectors consist of covariate vector of additive components for each subject.

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optnAdd A list of options controls B-spline parameters for additive components, specified

by list(name=value). See 'Details'.

optnVc A list of options controls B-spline parameters for varying-coefficient compo-

nents, specified by list(name=value). See 'Details'.

#### **Details**

VCAM provides a simple algorithm based on B-spline basis to estimate its nonparametric additive and varying-coefficient components.

Available control options for optnAdd are

**nKnot** A *d*-dimensional vector which designates the number of knots for each additive component function estimation (default=10).

**order** A *d*-dimensional vector which designates the order of B-spline basis for each additive component function estimation (default=3).

**grid** A N by d matrix whose column vector consist of evaluation grid points for each component function estimation.

and control options for optnVc are

**nKnot** A (d+1)-dimensional vector which designates the number of knots for overall mean function and each varying-coefficient component function estimation (default=10).

**order** A (d+1)-dimensional vector which designates the order of B-spline basis for overall mean function and each varying-coefficient component function estimation (default=3).

**grid** A M by (d+1) matrix whose column vectors consist of evaluation grid points for overall mean function and each varying-coefficient component function estimation.

#### Value

A list containing the following fields:

Lt The same with input given by *Lt*LyHat Fitted values corresponding to *Ly*phiEst An *N* by *d* matrix whose column vectors consist of estimates for each additive component function evaluated at *gridX*.

beta@Est An *M*-dimensional vector for overall mean function estimates evaluated at *gridT*.

betaEst An *M* by *d* matrix whose column vectors consist of estimates for each varying-coefficient components evaluated at *gridT*.

gridX The same with input given by *optnAdd\$grid* 

The same with input given by optnVc\$grid

### References

gridT

Zhang, X. and Wang, J.-L. (2015), "Varying-coefficient additive models for functional data", Biometrika, Vol.102, No.1, p.15-32.

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```
library(MASS)
set.seed(100)
n <- 100
d <- 2
Lt <- list()
Ly <- list()
m < - rep(0,2)
S \leftarrow matrix(c(1,0.5,0.5,1),nrow=2,ncol=2)
X <- pnorm(mvrnorm(n,m,S))</pre>
beta0 <- function(t) 1.5*sin(3*pi*(t+0.5))
beta1 <- function(t) 3*(1-t)^2
beta2 <- function(t) 4*t^3
phi1 <- function(x) sin(2*pi*x)</pre>
phi2 <- function(x) 4*x^3-1
for (i in 1:n) {
 Ni <- sample(10:20,1)
  Lt[[i]] <- sort(runif(Ni,0,1))
  Ly[[i]] <- beta0(Lt[[i]]) +
     beta1(Lt[[i]])*phi1(X[i,1]) + beta2(Lt[[i]])*phi2(X[i,2]) + rnorm(Ni,0,0.1)
}
vcam <- VCAM(Lt,Ly,X)</pre>
op <- par(no.readonly = TRUE)
par(mfrow=c(1,1))
plot(unlist(vcam$LyHat),unlist(Ly),xlab='observed Y',ylab='fitted Y')
abline(coef=c(0,1),col=8)
par(mfrow=c(1,2))
plot(vcam$gridX[,1],vcam$phiEst[,1],type='l',ylim=c(-1,1),xlab='x1',ylab='phi1')
points(vcam$gridX[,1],phi1(vcam$gridX[,1]),col=2,type='l',lty=2,lwd=2)
legend('topright',c('true','est'),lwd=2,lty=c(1,2),col=c(1,2))\\
plot(vcam$gridX[,2],vcam$phiEst[,2],type='l',ylim=c(-1,3),xlab='x2',ylab='phi2')
points(vcam$gridX[,2],phi2(vcam$gridX[,2]),col=2,type='1',lty=2,lwd=2)
legend('topleft', c('true', 'est'), lwd=2, lty=c(1,2), col=c(1,2))
par(mfrow=c(1,3))
plot(vcam$gridT,vcam$beta0Est,type='l',xlab='t',ylab='beta0')
points(vcam$gridT,beta0(vcam$gridT),col=2,type='1',lty=2,lwd=2)
```

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```
legend('topright',c('true','est'),lwd=2,lty=c(1,2),col=c(1,2))
plot(vcam$gridT,vcam$betaEst[,1],type='l',xlab='t',ylab='beta1')
points(vcam$gridT,beta1(vcam$gridT),col=2,type='l',lty=2,lwd=2)
legend('topright',c('true','est'),lwd=2,lty=c(1,2),col=c(1,2))
plot(vcam$gridT,vcam$betaEst[,2],type='l',xlab='t',ylab='beta2')
points(vcam$gridT,beta2(vcam$gridT),col=2,type='l',lty=2,lwd=2)
legend('topright',c('true','est'),lwd=2,lty=c(1,2),col=c(1,2))
par(op)
```

WFDA

Time-Warping in Functional Data Analysis: Pairwise curve synchronization for functional data

### **Description**

Time-Warping in Functional Data Analysis: Pairwise curve synchronization for functional data

### Usage

```
WFDA(Ly, Lt, optns = list())
```

### **Arguments**

Ly A list of *n* vectors containing the observed values for each individual.

Lt A list of *n* vectors containing the observation time points for each individual

corresponding to y. Each vector should be sorted in ascending order.

optns A list of options control parameters specified by list(name=value). See 'De-

tails'.

### Details

WFDA uses a pairwise warping method to obtain the desired alignment (registration) of the random trajectories. The data has to be regular. The routine returns the aligned curves and the associated warping function.

Available control options are

choice Choice of estimating the warping functions ('weighted' or 'truncated'). If 'weighted' then weighted averages of pairwise warping functions are computed; the weighting is based on the inverse pairwise distances. If 'truncated' the pairs with the top 10% largest distances are truncated and the simple average of the remaining pairwise distances are used - default: 'truncated'

**subsetProp** Pairwise warping functions are determined by using a subset of the whole sample; numeric (0,1] - default: 0.50

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**lambda** Penalty parameter used for estimating pairwise warping functions; numeric - default : V\*10^-4, where V is the average L2 norm of y-mean(y).

**nknots** Number of knots used for estimating the piece-wise linear pairwise warping functions; numeric - default: 2

**isPWL** Indicator if the resulting warping functions should piece-wise linear, if FALSE 'nknots' is ignored and the resulting warping functions are simply monotonic; logical - default: TRUE (significantly larger computation time.)

seed Random seed for the selection of the subset of warping functions; numeric - default: 666

**verbose** Indicator if the progress of the pairwise warping procedure should be displayed; logical - default: FALSE

### Value

A list containing the following fields:

optns Control options used.

lambda Penalty parameter used.

aligned Aligned curves evaluated at time 't'
h Warping functions for 't'

Inverse warping functions evaluated

hInv Inverse warping functions evaluated at 't' costs The mean cost associated with each curve

timing The time required by time-warping.

### References

Tang, R. and Müller, H.G. (2008). "Pairwise curve synchronization for functional data." Biometrika 95, 875-889

Tang, R. and Müller, H.G. (2009) "Time-synchronized clustering of gene expression trajectories." Biostatistics 10, 32-45

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```
+ rnorm(M, mean=0.0, sd= eps)
}

Y = as.list(as.data.frame(t(yMat)))
X = rep(list(T),N)

sss = WFDA(Ly = Y, Lt = X, list( choice = 'weighted' ))
op <- par(mfrow=c(1,2))
matplot(x= T, t(yMat), t='l', main = 'Raw', ylab = 'Y'); grid()
matplot(x= T, t(sss$aligned), t='l', main = 'Aligned', ylab='Y'); grid()
par(op)</pre>
```

Wiener

Simulate a standard Wiener processes (Brownian motions)

### **Description**

Simulate n standard Wiener processes on [0, 1], possibly sparsifying the results.

### Usage

```
Wiener(n = 1, pts = seq(0, 1, length = 50), sparsify = NULL, K = 50)
```

### **Arguments**

n	Sample size.	
pts	A vector of points in [0, 1] specifying the support of the processes.	
sparsify	A vector of integers. The number of observations per curve will be uniform distribution on sparsify.	
K	The number of components.	

#### **Details**

The algorithm is based on the Karhunen-Loève expansion of the Wiener process

# Value

If sparsify is not specified, a matrix with n rows corresponding to the samples are returned. Otherwise the sparsified sample is returned.

### See Also

Sparsify

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