

# Package ‘face’

January 19, 2018

**Title** Fast Covariance Estimation for Sparse Functional Data

**Version** 0.1-4

**Author** Luo Xiao [aut,cre], Cai Li [aut], William Checkley [aut], Ciprian Crainiceanu [aut]

**Maintainer** Luo Xiao <l Xiao5@ncsu.edu>

**Description** Implementation of the Fast Covariance Estimation for Sparse Functional Data paper published in Statistics and Computing, Xiao et al. (2018) <doi:10.1007/s11222-017-9744-8>.

**Depends** R (>= 2.1.4)

**Imports** stats, splines, Matrix, matrixcalc, mgcv, refund

**License** GPL-3

**LazyLoad** yes

**LazyData** true

**Repository** CRAN

**NeedsCompilation** no

**Date/Publication** 2018-01-19 15:05:12 UTC

## R topics documented:

face-package . . . . .	2
cor.face . . . . .	2
face-internal . . . . .	3
face.sparse . . . . .	3
predict.face.sparse . . . . .	8
predict.pspline.face . . . . .	9
pspline . . . . .	10
select.knots . . . . .	12

<b>Index</b>	<b>13</b>
--------------	-----------

---

face-package            *face*

---

### Description

Fast Covariance Estimation for Sparse Functional Data

### Details

Package:	face
Type:	Package
Version:	0.1-3
Date:	2017-03-30
License:	GPL-3

### Author(s)

Luo Xiao, Cai Li, William Checkley and Ciprian Crainiceanu

Maintainer: Luo Xiao <lxiao5@ncsu.edu>

### References

Luo Xiao, Cai Li, William Checkley and Ciprian Crainiceanu, Fast covariance estimation for sparse functional data, Stat. Comput., doi: [10.1007/s1122201797448](https://doi.org/10.1007/s1122201797448).

---

cor.face                    *Extraction of correlation and mean from a face.sparse object*

---

### Description

Extraction of correlation and mean from a face.sparse object

### Usage

```
cor.face(object, argvals.new, option="raw")
```

### Arguments

object	A face.sparse object.
argvals.new	Where to evaluate correlation and mean.
option	Defaults to "raw"; if "smooth", then extract correlation from smoothed covariance function.

**Value**

argvals.new	Where to evaluate correlation and mean.
option	Defaults to "raw"; if "smooth", then extract correlation from smoothed covariance function.
Cor	estimated correlation matrix at argvals.new
mu	estimated group/population mean at argvals.new

**Author(s)**

Luo Xiao <lxiao5@ncsu.edu>

**References**

Luo Xiao, Cai Li, William Checkley and Ciprian Crainiceanu, Fast covariance estimation for sparse functional data, Stat. Comput., doi: [10.1007/s1122201797448](https://doi.org/10.1007/s1122201797448).

**Examples**

```
# See the examples for "face.sparse".
```

---

face-internal	<i>Internal functions for face package</i>
---------------	--

---

**Description**

Internal function.

---

face.sparse	<i>Fast covariance estimation for sparse functional data</i>
-------------	--

---

**Description**

The function is to estimate the mean and covariance function from a cluster of functions/longitudinal observations.

**Usage**

```
face.sparse(data, newdata = NULL,
            center = TRUE, argvals.new = NULL,
            knots = 7,
            p = 3, m = 2, lambda = NULL, lambda_mean = NULL,
            search.length = 14,
            lower = -3, upper = 10, lower2 = -3, upper2 = 5,
            calculate.scores = FALSE, pve=0.99, two_step=FALSE)
```

**Arguments**

<code>data</code>	a data frame with three arguments: (1) <code>argvals</code> : observation times; (2) <code>subj</code> : subject indices; (3) <code>y</code> : values of observations. Missing values not allowed.
<code>newdata</code>	of the same structure as <code>data</code> ; defaults to <code>NULL</code> , then no prediction.
<code>center</code>	logical. If <code>TRUE</code> , then P-spline smoothing of the population mean will be conducted and subtracted from the data before covariance smoothing; if <code>FALSE</code> , then the population mean will be just 0s.
<code>argvals.new</code>	a vector of observation time points to evaluate mean function, covariance function, error variance and etc. If <code>NULL</code> , then 100 equidistant points in the range of <code>data\$argvals</code> .
<code>knots</code>	the number of knots for B-spline basis functions to be used; defaults to 7. The resulting number of basis functions is the number of interior knots plus the degree of B-splines.
<code>p</code>	the degrees of B-splines; defaults to 3.
<code>m</code>	the order of differencing penalty; defaults to 2.
<code>lambda</code>	the value of the smoothing parameter for covariance smoothing; defaults to <code>NULL</code> .
<code>lambda.mean</code>	the value of the smoothing parameter for mean smoothing; defaults to <code>NULL</code> .
<code>search.length</code>	the number of equidistant (log scale) smoothing parameters to search; defaults to 14.
<code>lower, upper</code>	bounds for log smoothing parameter for first step of estimation; defaults are -3 and 10, respectively.
<code>lower2, upper2</code>	bounds for log smoothing parameter for second step of estimation; defaults are lower and 5, respectively.
<code>calculate.scores</code>	if <code>TRUE</code> , scores will be calculated.
<code>pve</code>	Defaults 0.99. To select the number of eigenvalues by percentage of variance.
<code>two_step</code>	if <code>TRUE</code> , a two-step estimation procedure will be applied.

**Details**

This is a generalized version of bivariate P-splines (Eilers and Marx, 2003) for covariance smoothing of sparse functional or longitudinal data. It uses tensor product B-spline basis functions and employs a differencing penalty on the associated parameter matrix. The only smoothing parameter in the method is selected by leave-one-subject-out cross validation and is implemented with a fast algorithm.

There are two steps for estimation. During the first step, the objective function to minimize is the penalized least squares on empirical estimates of covariance function. During the second step, the covariance between the empirical estimates (depending on the estimates of covariance function) are accounted and thus a generalized penalized least squares are minimized.

If `center` is `TRUE`, then a population mean will be calculated and is smoothed by univariate P-spline smoothing: `pspline` (Eilers and Marx, 1996). This univariate smoothing uses leave-one-subject-out cross validation to select the smoothing parameter.

The knots are "equally-spaced", the differencing penalty in Eilers and Marx (2003) is used.

If the functional data are observed at the same grid for each function/curve and can be organized into a data matrix, then `fpca.face` in the package `refund` should instead be used. `fpca.face` allows a small percentage (less than 30 percent) of missing data in the data matrix.

### Value

<code>newdata</code>	Input
<code>y.pred</code> , <code>mu.pred</code> , <code>Chat.diag.pred</code> , <code>var.error.pred</code>	Predicted/estimated objects at <code>newdata\$argvals</code>
<code>Theta</code>	Estimated parameter matrix
<code>argvals.new</code>	Vector of time points to evaluate population parameters
<code>mu.new</code> , <code>Chat.new</code> , <code>Cor.new</code> , <code>Cor.raw.new</code> , <code>Chat.raw.diag.new</code> , <code>var.error.new</code>	Estimated objects at <code>argvals.new</code>
<code>eigenfunctions</code> , <code>eigenvalues</code>	Estimated eigenfunctions (scaled eigenvector) and eigenvalues at <code>argvals.new</code>
<code>mu.hat</code> , <code>var.error.hat</code>	Estimated objects at <code>data\$argvals</code>
<code>calculate.scores</code> , <code>scores</code>	if <code>calculate.scores</code> is TRUE (default to FALSE) and <code>newdata</code> is not NULL, then predicted scores will be calculated.
...	...

### Author(s)

Luo Xiao <lxiao5@ncsu.edu> and Cai Li <cli9@ncsu.edu>

### References

Luo Xiao, Cai Li, William Checkley and Ciprian Crainiceanu, Fast covariance estimation for sparse functional data, *Stat. Comput.*, doi: [10.1007/s1122201797448](https://doi.org/10.1007/s1122201797448).

Paul Eilers and Brian Marx, Multivariate calibration with temperature interaction using two-dimensional penalized signal regression, *Chemometrics and Intelligent Laboratory Systems* 66 (2003), 159-174.

Paul Eilers and Brian Marx, Flexible smoothing with B-splines and penalties, *Statist. Sci.*, 11, 89-121, 1996.

Simon N. Wood, P-splines with derivative based penalties and tensor product smoothing of unevenly distributed data, *Stat. Comput.*, doi: [10.1007/s112220169666x](https://doi.org/10.1007/s112220169666x).

### See Also

`fpca.face` and `fpca.sc` in `refund`

## Examples

```

## Not run:
#####
#### CD4 data example
#####

require(refund)
data(cd4)
n <- nrow(cd4)
T <- ncol(cd4)

id <- rep(1:n,each=T)
t <- rep(-18:42, times=n)
y <- as.vector(t(cd4))
sel <- which(is.na(y))

## organize data and apply FACEs
data <- data.frame(y=log(y[-sel]),
  argvals = t[-sel],
  subj = id[-sel])
data <- data[data$y>4.5,]
fit_face <- face.sparse(data, argvals.new=(-20:40))

data.h <- data
tnew <- fit_face$argvals.new

## scatter plots
Xlab <- "Months since seroconversion"
Ylab <- "log (CD4 count)"
par(mfrow=c(1,1),mar = c(4.5,4.5,3,2))
id <- data.h$subj
uid <- unique(id)
plot(data.h$argvals,data.h$y,
  type = "n", ylim = c(4.5,8),
  xlab = Xlab, ylab = Ylab,
  cex.lab = 1.25,cex.axis=1.25,cex.main = 1.25)

for(i in 1:10){
  seq <- which(id==uid[i])
  lines(data.h$argvals[seq],data.h$y[seq],lty=1,col="gray",lwd=1,type="l")
  #points(data.h$argvals[seq],data.h$y[seq],col=1,lty=1,pch=1)
}

Sample <- seq(10,50,by=10)
for(i in Sample){
  seq <- which(id==uid[i])
  lines(data.h$argvals[seq],data.h$y[seq],lty=1,col="black",lwd=1,type="l")
}
lines(tnew,fit_face$mu.new,lwd=2,lty=2,col="red")

```

```

## plots of variance/correlation functions

Cov <- fit_face$Chat.new
Cov_diag <- diag(Cov)
Cor <- fit_face$Cor.new

par(mfrow=c(1,2),mar=c(4.5,4.1,3,4.5))

plot(tnew,Cov_diag,type="l",
     xlab = Xlab, ylab="",main= "CD4: variance function",
     #ylim = c(0.8,1.5),
     cex.axis=1.25,cex.lab=1.25,cex.main=1.25,lwd=2)

require(fields)
image.plot(tnew,tnew,Cor,
           xlab=Xlab, ylab = Xlab,
           main = "CD4: correlation function",
           cex.axis=1.25,cex.lab=1.25,cex.main=1.25,
           axis.args = list(at = c(0,0.2,0.4,0.6,0.8,1.0)),
           legend.shrink=0.75,legend.line=-1.5)

## prediction of several subjects

par(mfrow=c(2,2),mar=c(4.5,4.5,3,2))
Sample <- c(30,40,50,60)
for(i in 1:4){
  sel <- which(id==uid[Sample[i]])
  dati <- data.h[sel,]

  seq <- -20:40
  k <- length(seq)
  dati_pred <- data.frame(y = rep(NA,nrow(dati) + k ),
                        argvals = c(rep(NA,nrow(dati)),seq),
                        subj=rep(dati$subj[1],nrow(dati) + k )
                        )

  dati_pred[1:nrow(dati),] <- dati
  yhat2 <- predict(fit_face,dati_pred)

  data3 <- dati
  Ylim <- range(c(data3$y,yhat2$y.pred))

  plot(data3$argvals,data3$y,xlab=Xlab,ylab=Ylab, main = paste("Male ",i,sep=""),
       ylim = c(4,8.5),
       cex.lab=1.25,cex.axis = 1.25,cex.main = 1.25,pch=1,xlim=c(-20,40))

  Ord <- nrow(dati) + 1:k
  lines(dati_pred$argvals[Ord],yhat2$y.pred[Ord],col="red",lwd=2)
  lines(dati_pred$argvals[Ord],
        yhat2$y.pred[Ord] - 1.96*yhat2$se.pred[Ord], col="red",lwd=1,lty=2)
  lines(dati_pred$argvals[Ord],

```

```

yhat2$y.pred[Ord] + 1.96*yhat2$se.pred[Ord], col="red",lwd=1,lty=2)

lines(tnew,fit_face$mu.new,lty=3,col="black",lwd=2)
legend("bottomleft",c("mean","prediction"),lty=c(3,1),col=1:2,lwd=2,bty="n")
}

## End(Not run)

```

---

predict.face.sparse     *Subject-specific curve prediction from a face.sparse fit*

---

### Description

Predict subject-specific curves based on a fit from "face.sparse".

### Usage

```
## S3 method for class 'face.sparse'
predict(object, newdata, ...)
```

### Arguments

object	a fitted object from the R function "face.sparse".
newdata	a data frame with three arguments: (1) argvals: observation times; (2) subj: subject indices; (3) y: values of observations. NA values are allowed in "y" but not in the other two.
...	further arguments passed to or from other methods.

### Details

This function makes prediction based on observed data for each subject. So for each subject, it requires at least one observed data. For the time points prediction is desired but no observation is available, just make the corresponding data\$y as NA.

### Value

object	A "face.sparse" fit
newdata	Input
y.pred,mu.pred,Chat.pred, Chat.diag.pred, var.error.pred	Predicted/estimated objects at the observation time points in newdata
scores	if calculate.scores in object is TRUE (typically FALSE), then predicted scores will be calculated.
...	...

### Author(s)

Luo Xiao <lxiao5@ncsu.edu>



## References

Luo Xiao, Cai Li, William Checkley and Ciprian Crainiceanu, Fast covariance estimation for sparse functional data, Stat. Comput., doi: [10.1007/s1122201797448](https://doi.org/10.1007/s1122201797448).

## Examples

```
#See the examples for "face.sparse".
```

---

`predict.pspline.face` *Mean prediction from a P-spline smoothing fit*

---

## Description

Predict mean values based on a fit from "pspline".

## Usage

```
## S3 method for class 'pspline.face'  
predict(object, argvals.new,...)
```

## Arguments

<code>object</code>	a fitted object from the R function "pspline".
<code>argvals.new</code>	a vector of new time points.
<code>...</code>	further arguments passed to or from other methods.

## Value

Predicted means at `argvals.new`.

## Author(s)

Luo Xiao <[lxiao5@ncsu.edu](mailto:lxiao5@ncsu.edu)>

## References

Luo Xiao, Cai Li, William Checkley and Ciprian Crainiceanu, Fast covariance estimation for sparse functional data, Stat. Comput., doi: [10.1007/s1122201797448](https://doi.org/10.1007/s1122201797448).

## Examples

```
#See the examples for "pspline".
```

pspline

*Univariate P-spline smoothing***Description**

Univariate P-spline smoothing with the smoothing parameter selected by leave-one-subject-out cross validation.

**Usage**

```
pspline(data, argvals.new = NULL, knots = 35,
        p = 3, m = 2, lambda = NULL,
        search.length = 100,
        lower = -20, upper = 20)
```

**Arguments**

data	a data frame with three arguments: (1) argvals: observation times; (2) subj: subject indices; (3) y: values of observations. Missing values not allowed.
argvals.new	a vector of observations times for prediction; if NULL, then the same as data\$argvals.
knots	a vector of interior knots or the number of knots for B-spline basis functions to be used; defaults to 35.
p	the degrees of B-splines; defaults to 3.
m	the order of differencing penalty; defaults to 2.
lambda	the value of the smoothing parameter; defaults to NULL.
search.length	the number of equidistant (log scale) smoothing parameters to search; defaults to 100.
lower, upper	bounds for log smoothing parameter; defaults are -20 and 20.

**Details**

The function is an implementation of the P-spline smoothing in Eilers and Marx (1996). P-splines uses B-splines as basis functions and employs a differencing penalty on the coefficients. Leave-one-subject-out cross validation is used for selecting the smoothing parameter and a fast algorithm is implemented.

**Value**

fitted.values	Fitted mean values
B	B-spline design matrix
theta	Estimated coefficients
s	Eigenvalues
knots	Knots
p	The degrees of B-splines

m	The order of differencing penalty
lambda	The value of the smoothing parameter
argvals.new	A vector of observations times
mu.new	Fitted mean values at argvals.new

**Author(s)**

Luo Xiao <lxiao5@ncsu.edu>

**References**

Paul Eilers and Brian Marx, Flexible smoothing with B-splines and penalties, *Statist. Sci.*, 11, 89-121, 1996.

Luo Xiao, Cai Li, William Checkley and Ciprian Crainiceanu, Fast covariance estimation for sparse functional data, *Stat. Comput.*, doi: [10.1007/s1122201797448](https://doi.org/10.1007/s1122201797448).

**See Also**

[gam](#) in [mgcv](#).

**Examples**

```
## cd4 data
require(refund)
data(cd4)
n <- nrow(cd4)
T <- ncol(cd4)

id <- rep(1:n,each=T)
t <- rep(-18:42, times=n)
y <- as.vector(t(cd4))
sel <- which(is.na(y))

## organize data
data <- data.frame(y=log(y[-sel]),
  argvals = t[-sel],
  subj = id[-sel])
data <- data[data$y>4.5,]

## smooth
fit <- pspline(data)

## plot
plot(data$argvals, fit$mu.new, type="p")

## prediction
pred <- predict(fit, quantile(data$argvals, c(0.2, 0.6)))
pred
```

---

select.knots	<i>Knots selection for P-spline smoothing</i>
--------------	---

---

**Description**

Construct knots from either quantiles of observed time points or equally-spaced time points.

**Usage**

```
select.knots(t,knots=10,p=3,option="equally-spaced")
```

**Arguments**

t	Observed time points.
knots	Number of interior knots.
p	Degrees of B-splines to be used.
option	Default "equally-spaced": equally-spaced time points in the range of t; if "quantile", then quantiles of t.

**Details**

The number of knots in the output will be knot plus 2 times p; and the B-spline basis matrix constructed from this vector of knots with degrees p will be knots plus p.

**Value**

A vector of knots

**Author(s)**

Luo Xiao <lxiao5@ncsu.edu>

**Examples**

```
t <- rnorm(100)
knots <- select.knots(t)
```

# Index

- \*Topic **\textasciitildePspline**
  - predict.pspline.face, 9
  - pspline, 10
  - select.knots, 12
- \*Topic **\textasciitildeface.sparse**
  - cor.face, 2
  - face.sparse, 3
  - predict.face.sparse, 8
- \*Topic **\textasciitildeprediction**
  - predict.face.sparse, 8
  - predict.pspline.face, 9
- \*Topic **package**
  - face-package, 2

check.data (face-internal), 3  
construct.knots (face-internal), 3  
cor.face, 2  
covZ (face-internal), 3

face (face-package), 2  
face-internal, 3  
face-package, 2  
face.sparse, 3  
face.sparse.inner (face-internal), 3

gam, 11

kr (face-internal), 3

matrix.multiply (face-internal), 3  
mgcv, 11

predict.face.sparse, 8  
predict.pspline.face, 9  
pspline, 10  
pspline.setting (face-internal), 3

raw.construct (face-internal), 3

select.knots, 12

weight.construct (face-internal), 3