STAT 597: Functional Data Analysis
Week 01 – Day 02 – Lecture 02
Chapter 1 – First Steps

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Outline

We continue with Chapter 1 - First steps.

- Mean functions
- Covariance functions
- Functional principal components
- Two examples

We will focus especially on how to use bases for various computations.

Data structure

Assume we have an iid sample of functions

$$X_n(t) \qquad n = 1, \ldots, N \qquad 0 \leq t \leq 1.$$

What does it mean to be iid? From here on, we will assume that we can construct these functions in `R` as fd objects.

Mean Function

Population level:

$$\mu(t) := \mathrm{E}[X_n(t)].$$

Sample level:

$$\widehat{\mu}(t) := \frac{1}{N} \sum_{n=1}^{N} X_n(t).$$

In later chapters, we will discuss asymptotic properties of $\widehat{\mu}(t)$.

Mean Function - Computation

We can use the basis expansion of $X_n(t)$ to do this computation fairly easily. Recall that

$$X_n(t) = \sum_m c_{nm} B_m(t).$$

So one has

$$\widehat{\mu}(t) = \frac{1}{N} \sum_n \sum_m c_{nm} B_m(t) = \sum_m \bar{c}_m B_m(t),$$

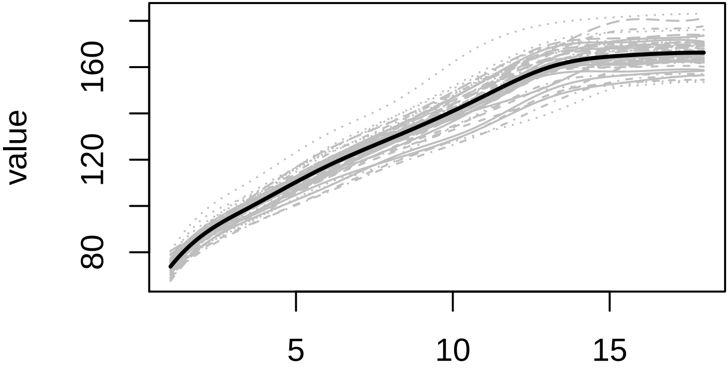
where

$$\bar{c}_m = \frac{1}{N} \sum_n c_{nm}.$$

As in univariate and multivariate statistics, we use the mean to summarize the center/average value of the data. We can also visualize how this value changes with time.

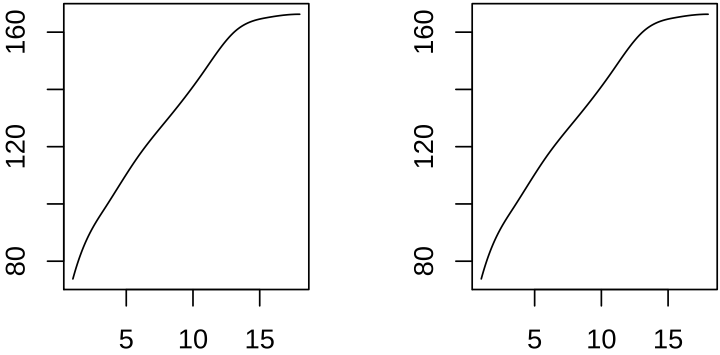
Mean Function - Berkeley Growth

```
times = growth$age; GHeight = growth$hgtf
my_basis<-create.bspline.basis(c(1,18),nbasis=10)
GHeight.F<-Data2fd(times,GHeight,my_basis)
mu.F<-mean.fd(GHeight.F)
plot(GHeight.F,col='grey'); plot(mu.F,lwd=2,add=TRUE)
```



Mean Function - Alt Calc

```
GHeight_coef<-GHeight.F$coefs
mean_coef<-rowMeans(GHeight_coef)
mu.F2<-fd(coef=mean_coef,basisobj=my_basis)
plot(mu.F,ylab="",xlab="");plot(mu.F2,ylab="",xlab="")
```



Covariance Function

Population level:

$$C(t,s) := \mathrm{E}[(X_n(t) - \mu(t))(X_n(s) - \mu(s))].$$

Sample level:

$$\widehat{C}(t,s) := \frac{1}{N-1}\sum_{n=1}^{N}(X_n(t) - \widehat{\mu}(t))(X_n(s) - \widehat{\mu}(s)).$$

In later chapters, we will discuss asymptotic properties of $\widehat{C}(t,s)$. As in multivariate statistics, C describes how the different time points covary, i.e. how dependent are your height today and 10 years ago?

Covariance Function - Computation

Let $\tilde{c}_{nm} = c_{nm} - \bar{c}_m$ be the centered coefficients and $\tilde{\mathbf{c}}$ be the matrix of centered coefficients. Then

$$\begin{aligned}
\widehat{C}(t,s) &= \frac{1}{N-1} \sum_n \sum_{m_1} \sum_{m_2} \tilde{c}_{nm_1} \tilde{c}_{nm_2} B_{m_1}(t) B_{m_2}(s) \\
&= \frac{1}{N-1} \sum_{m_1} \sum_{m_2} (\tilde{\mathbf{c}}^\top \tilde{\mathbf{c}})_{m_1,m_2} B_{m_1}(t) B_{m_2}(s) \\
&= \sum_{m_1} \sum_{m_2} (\boldsymbol{\Sigma}_c)_{m_1 m_2} B_{m_1}(t) B_{m_2}(s).
\end{aligned}$$

So $\widehat{C}(t,s)$ can be expressed using a basis expansion. The basis $\{B_{m_1}(t)B_{m_2}(s) : m_1 = 1, \ldots, M, \; m_2 = 1, \ldots, M\}$ is called a *tensor basis*. The coefficients are given by $(N-1)\mathbf{c}^\top \mathbf{c}$.

Covariance Function - bifd

```
GHeight_var<-var.fd(GHeight.F)
class(GHeight_var)

## [1] "bifd"

names(GHeight_var)

## [1] "coefs"     "sbasis"    "tbasis"    "bifdnames"

dim(GHeight_var$coefs)

## [1] 10 10
```

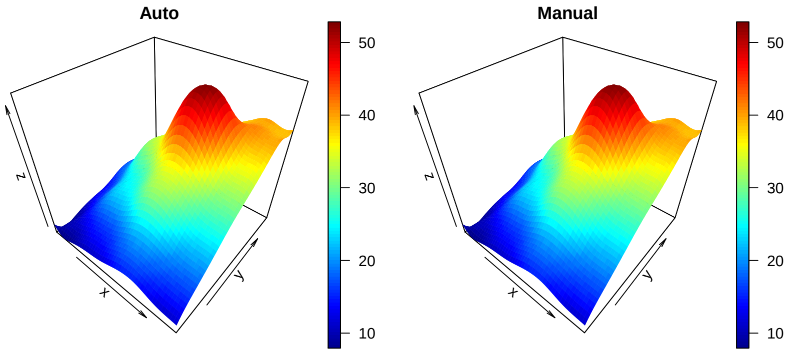
The covariance function is a *bivariate functional object* in R. *coefs* can be 2,3, or 4 dimensional. If it is 2, then R understands there is only one bifd object. If it is 3, then R understands that there is a sample of bifd objects (4 dimensions corresponds to multiple variables).

Covariance Function - Manual

```
# Manual
coef_mat<-coef(GHeight.F); N<-dim(coef_mat)[2]
coef_mean<-rowMeans(coef_mat)
coef_center<-sweep(coef_mat,1,coef_mean)
C_hat_coef<-(coef_center%*%t(coef_center))/(N-1)
C_hat<-bifd(coef=t(C_hat_coef),sbasisobj = my_basis,
            tbasisobj = my_basis)
```

Warning: Remember that the `fda` package assumes that different curves correspond to different collumns in the coefficient matrix (the transpose of how we defined **c**).

Covariance Function - Manual vs Auto



Functional Principal Components

As was mentioned, Principal Components are the eigenfunctions (vectors) of the covariance function (matrix). These are a cornerstone of FDA and multivariate statistics, so we will give them more attention later on. An eigenvalue/function pair (λ_j, v_j) satisfies

$$\text{Population:} \quad \lambda_j v_j(t) = \int_0^1 C(t,s) v_j(s)\, ds \quad \text{with} \quad \int v_j(t)^2\, dt = 1.$$

$$\text{Sample:} \quad \hat{\lambda}_j \hat{v}_j(t) = \int_0^1 \widehat{C}(t,s) \hat{v}_j(s)\, ds \quad \text{with} \quad \int \hat{v}_j(t)^2\, dt = 1.$$

More details/theory on this later.

FPCA - Calc

These next steps are a lot easier if $B_m(t)$ satisfy:

$$\int B_{m_1}(t) B_{m_2}(t)\ dt = 1_{m_1 = m_2}.$$

So we will assume this for a few slides (called orthonormal). If we expand $v_j(t)$ using the $B_j(t)$:

$$v_j(t) = \sum_m v_{jm} B_m(t),$$

then we can obtain a set of linear equations involving $\mathbf{v}_j = \{v_{jm}\}$ by integrating against $B_m(t)$:

$$\lambda_j \int v_j(t) B_{m_1}(t)\ dt = \int_0^1 \int_0^1 C(t,s) v_j(s) B_{m_1}(t)\ ds\ dt.$$

Notice that

$$\lambda_j \int v_j(t) B_{m_1}(t) = \lambda_j \sum_{m_2} v_{jm_2} \int B_{m_1}(t) B_{m_2}(t)\ dt = \lambda_j v_{jm_1}.$$

FPCA - Calc (cont)

We also have that

$$\int_0^1 \int_0^1 C(t,s) v_j(s) B_{m_1}(t)$$
$$= \sum_{m_2} \sum_{m_3} (\boldsymbol{\Sigma}_c)_{m_2 m_3} \int B_{m_2}(t) B_{m_1}(t) \; dt \int B_{m_3}(s) v_j(s) \; ds$$
$$= \sum_{m_3} (\boldsymbol{\Sigma}_c)_{m_1 m_3} v_{j m_3}.$$

So the coefficients, $\mathbf{v}_j$, for the eigenfuncion v_j, satisfies

$$\lambda_j \mathbf{v}_j = \boldsymbol{\Sigma}_c \mathbf{v}_j \quad \text{and} \quad \mathbf{v}_j^\top \mathbf{v}_j = 1.$$

FPCA - Nonorthonormal basis

If the $B_m(t)$ are not orthonormal, then the equations are a bit uglier. However, any basis can be made orthogonal via some linear (matrix) transoformation $\mathbf{W}$, that is

$$\tilde{B}_m(t) = \sum_{m_1} W_{mm_1} B_m(t),$$

are an orthonormal basis. This then implies that

$$\begin{aligned} v_j(t) = \sum_m v_{jm} B_m(t) &= \sum_m v_{jm} \sum_{m_1} (\mathbf{W}^{-1})_{mm_1} \tilde{B}_{m_1}(t) \\ &= \sum_{m_1} (\mathbf{W}^{-1}\mathbf{v})_{m_1} \tilde{B}_{m_1}(t). \end{aligned}$$

And so $\mathbf{W}$ provides a change of basis transformation $\tilde{\mathbf{v}}_j = \mathbf{W}^{-1}\mathbf{v}_j$.

FPCA - Nonorthonormal basis - Cont

Similar arguments show that

$$\widetilde{\boldsymbol{\Sigma}}_c = \mathbf{W}^{-1}\boldsymbol{\Sigma}_c\mathbf{W}^{-1},$$

and we therefore have the relation

$$\lambda_j \tilde{\mathbf{v}}_j = \widetilde{\boldsymbol{\Sigma}}_c \tilde{\mathbf{v}}_j \text{ and } \lambda_j \mathbf{W}^{-1}\mathbf{v}_j = \mathbf{W}^{-1}\boldsymbol{\Sigma}_c\mathbf{W}^{-2}\mathbf{v}_j$$
$$\text{with } \mathbf{v}_j^\top \mathbf{W}^{-2}\mathbf{v}_j = 1.$$

FPCA in R

```
GHeight_pc<-pca.fd(GHeight.F,nharm=3)
class(GHeight_pc)

## [1] "pca.fd"

names(GHeight_pc)[1:3]; names(GHeight_pc)[4:5]

## [1] "harmonics" "values"    "scores"
## [1] "varprop" "meanfd"
```

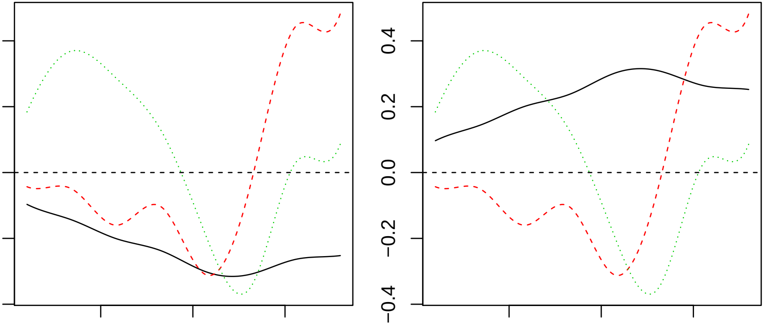
- *nharm*: the number of desired pcs
- *harmonics*: these are the principal components
- *values*: these are the eigenvalues
- *scores*: these are the coefficients in the basis expansion
- *varprop*: these are the explained variances for each pc
- *meanfd*: mean function of the data

FPCA in R - manual

```
library(expm);
W2inv<-inprod(my_basis,my_basis);
Sig_c<-cov(t(coef_mat)); A<-Sig_c%*%W2inv
e_A<-eigen(A)
names(e_A)

## [1] "values"  "vectors"

e_A$values[1:3]

## [1] 493.16109  35.23920  14.03662

GHeight_pc$values[1:3]

## [1] 484.02773  34.58686  13.77659
```

FPCA in R - manual (cont)

```
v_coef<-e_A$vectors[,1:3]
norm_v<-diag(t(v_coef)%*%W2inv%*%v_coef)
v_coef<-v_coef%*%diag(1/sqrt(norm_v))
e_fun<-fd(v_coef,my_basis)
plot(e_fun); plot(GHeight_pc$harmonics)

## [1] "done"
```



FPCA - Scores

A primary use of FPCA is dimension reduction. High/infinite dimensional ojbects can be represented using a fairly small number of FPCs:

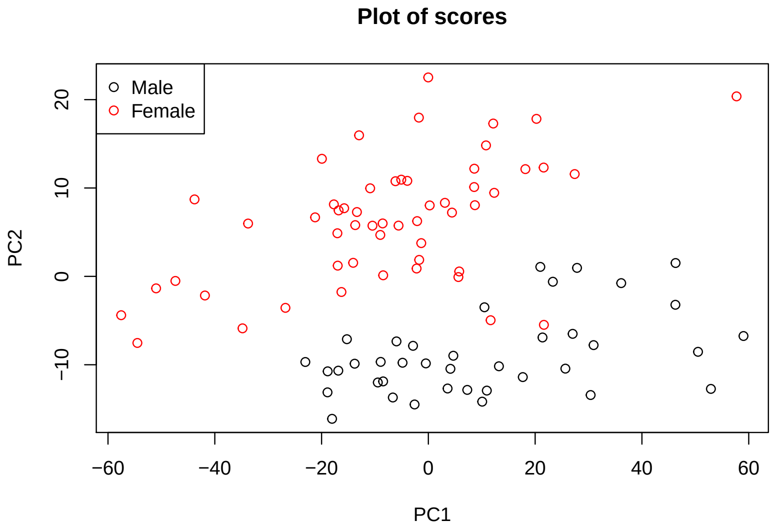
$$X_n(t) - \bar{X}(t) \approx \sum_{j=1}^{p} \hat{\xi}_{nj} \hat{v}_j(t),$$

where

$$\hat{\xi}_{nj} = \int (X_n(t) - \bar{X}(t)) \hat{v}_j(t).$$

These scores can be used for a variety of purposes. Sometimes we just can't work with infinite dimensional objects. At other times, the scores may prove useful to examine.

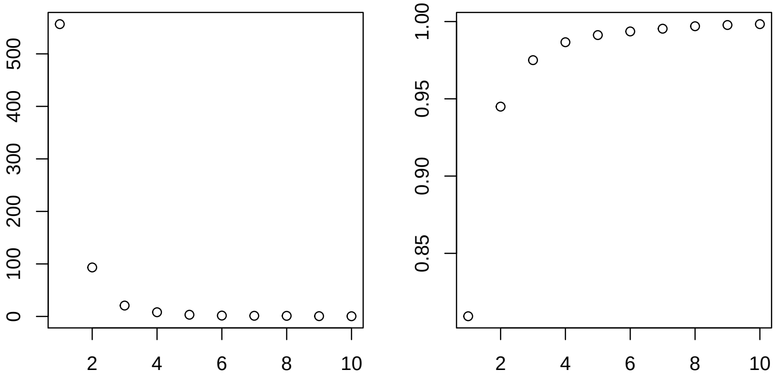
FPCA - Scores - Berkeley, both genders



FPCA - Explained Variance - Berkeley

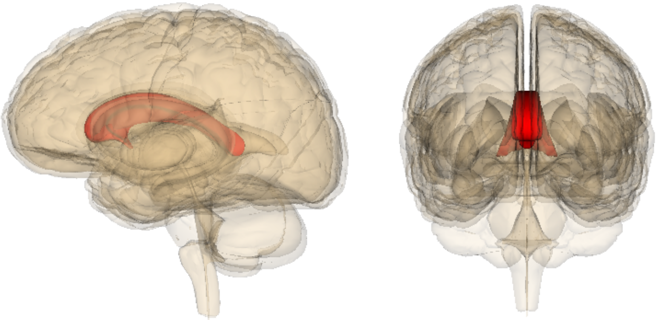
The first p eigenfunctions explain the following proportion of variance

$$\sum_{j=1}^{p} \lambda_j / \sum_{j=1}^{\infty} \hat{\lambda}_j.$$



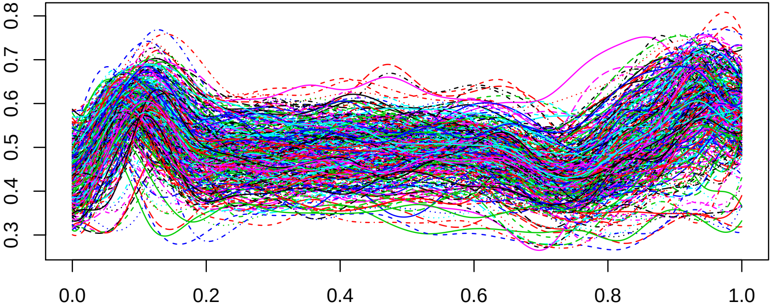
Diffusion Tensor Imaging

The DTI dataset is part of the `refund` package in `R`. This package is mainly composed of tools for functional regression. The data consists of scans of certain white matter tracts in the brain. The one we consisder here is called the *corpus callosum*, a white matter tract which connects the two hemispheres of the brain. The data was collected as part of a study on Multiple Sclerosis and its affect on the brain. Note:"The MRI/DTI data were collected at Johns Hopkins University and the Kennedy-Krieger Institute"



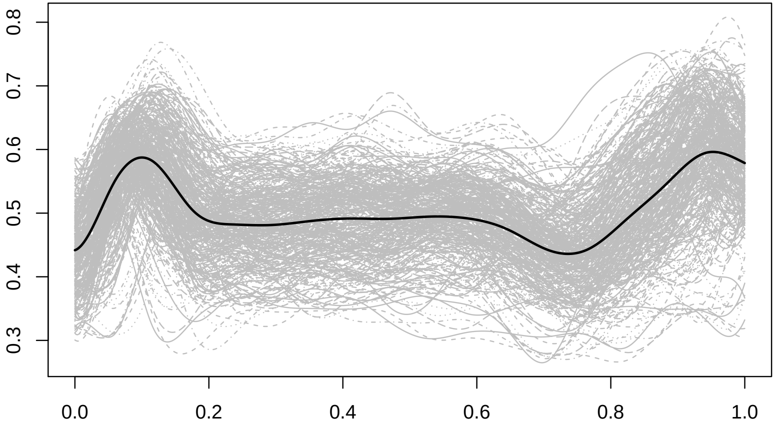
Diffusion Tensor Imaging

```
Corp<-DTI$cca
drop<-unique(which(is.na(Corp),arr.ind=TRUE)[,1])
Corp<-Corp[-drop,] # Missing value
pts<-seq(0,1,length=93)
my_basis<-create.bspline.basis(c(0,1),nbasis=20)
Corp.F<-Data2fd(pts,t(Corp),my_basis)
plot(Corp.F)
```



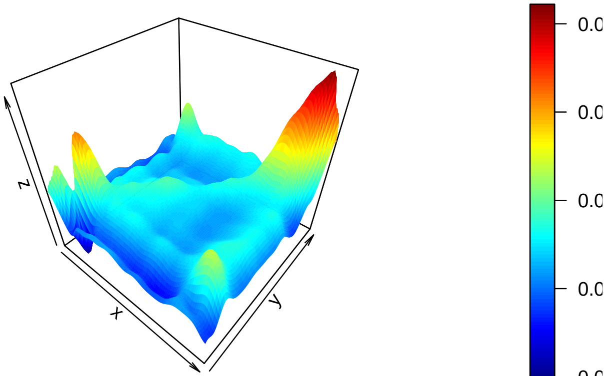
DTI-Mean

```
plot(Corp.F,col="gray")
Corp.F.mean<-mean(Corp.F)
plot(Corp.F.mean,add=TRUE,lwd=2)
```



DTI-Covariance

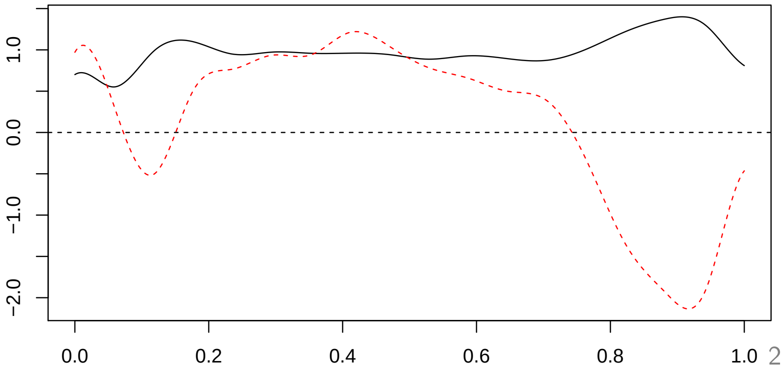
```
Cov_DTI<-var.fd(Corp.F)
pts<-seq(0,1,length=100)
Cov_DTI_mat<-eval.bifd(pts,pts,Cov_DTI)
persp3D(pts,pts,Cov_DTI_mat)
```



DTI-FPCA

```
DTI_pc<-pca.fd(Corp.F,nharm=2)
DTI_pc$varprop

## [1] 0.64858233 0.08276098
```

```
plot(DTI_pc$harmonics)
```



DTI-FPCA as an approximation

```
DTI_e_fun<-DTI_pc$harmonics
DTI_scores<-DTI_pc$scores
dim(DTI_scores)
approx_fun<-Corp.F.mean+DTI_e_fun[1]*DTI_scores[1,1]+
  DTI_e_fun[2]*DTI_scores[1,2]
plot(Corp.F[1]); plot(approx_fun,add=TRUE,lty=2)
```