STAT 597: Functional Data Analysis
Lecture 3 – Chapter 2 – Further topics

Instructor: Matthew Reimherr

Outline

We begin Chapter 2 - Further topics.

- Derivatives
- Penalized Smoothing
- Curve Alignment

Derivatives

The ability to examine derivatives is another distinction of FDA (as compared to MVA). Once a function, $X_n(t)$ is represented using a basis, calculating its derivative is relatively straightfoward.

$$X_n(t) = \sum_{k=1}^{K} c_{nk} B_k(t) \Longrightarrow X_n'(t) = \sum_k c_{nk} B_k'(t).$$

(if the sum is finite, this is trivially true, what if the sum is infinite?)

Example - Matérn

The Matérn process is a Gaussian process with covariance function is defined as

$$C(t,s) = \sigma^2 \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\sqrt{2\nu} \frac{|t-s|}{\rho} \right) K_\nu \left(\sqrt{2\nu} \frac{|t-s|}{\rho} \right)$$

- σ^2 : Point-wise variance.
- ρ: Range parameter, controls how quickly dependence falls off.
- ν: Smoothness parameter, controls number of derivatives of resulting process ($< \nu - 1$).
- K_ν: Bessel function of the second kind.

A good process for simulating "realistic" data. Popular in spatial statistics.

Example - Matérn

A few examples.

- If $\nu = 1/2$ then

$$C(t,s) = \sigma^2 \exp\{-|t-s|/\rho\}.$$

- If $\nu = 3/2$ then

$$C(t,s) = \sigma^2 \left(1 + \sqrt{3}|t-s|/\rho\right) \exp\{-\sqrt{3}|t-s|/\rho\}.$$

- If $\nu = \infty$ then

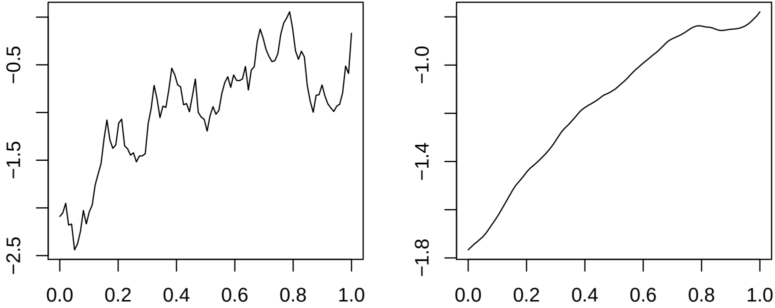
$$C(t,s) = \sigma^2 \exp\{-|t-s|^2/(2\rho^2)\}$$

The top one has a special name, what is it?

Example - Matérn - Code

```
set.seed(201609); library(fields); library(expm)
m<-100; times<-seq(0,1,length=m)
range<-1; nu1=1/2; sig2<-1; nu2=3/2
Matern(.5,range=range,nu=nu1)

## [1] 0.6065307

d_mat<-abs(outer(times,times,"-"))
C_1<-apply(d_mat,c(1,2),FUN=Matern,range=range,nu=nu1)
C_1<-C_1*sig2
C_1_sq<-sqrtm(C_1)
C_2<-apply(d_mat,c(1,2),FUN=Matern,range=range,nu=nu2)
C_2<-C_2*sig2
C_2_sq<-sqrtm(C_2)
Z<-rnorm(m)
X1<-C_1_sq%*%Z; X2<-C_2_sq%*%Z
```

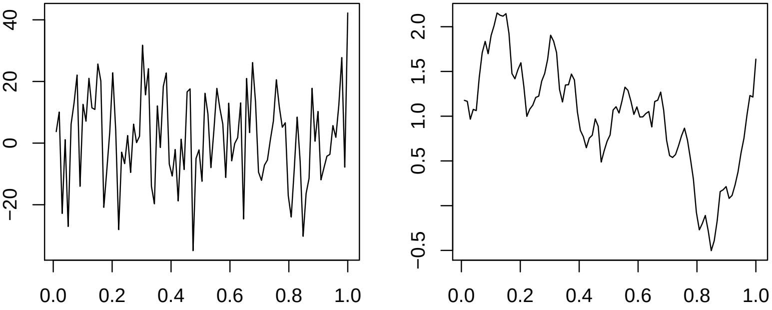
Example - Matérn - Plot



Example - Numeric Derivative

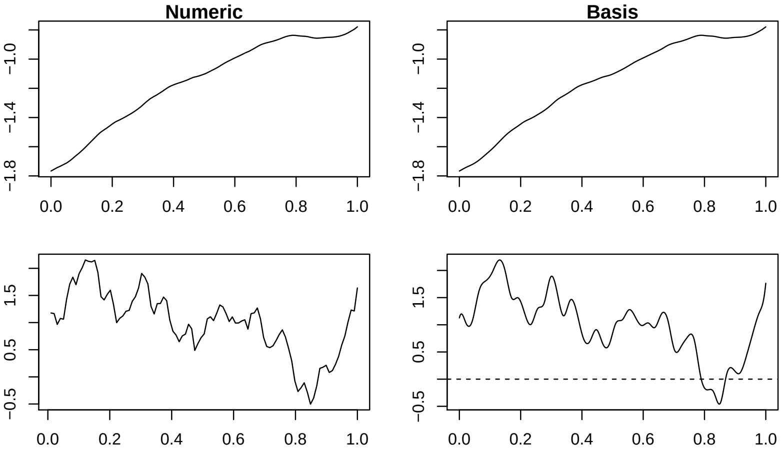
If we observe $\{X(t_i)\}$ then we can approximate its derivative:

$$X'(t_i) \approx \frac{X(t_i) - X(t_{i-1})}{t_i - t_{i-1}}.$$



Example - Compare

```
mybasis<-create.bspline.basis(c(0,1),nbasis=50)
X2.f<-Data2fd(times,X2,mybasis)
X2d.f<-deriv.fd(X2.f)
```



Penalized smoothing

Taking derivatives of functions must be done with care. If the data hasn't been properly smoothed then the functions can look funny or be misleading. We will now develop a strategy for more carefully smoothing the curves. As a by product, the choice of the number of basis functions will no longer be too crucial (as long as it is relatively large).

Suppose that $\{Y_{jn}\}$ are the function vaues observed at time points t_{nj}. Our aim is to reconstruct $X_n(t)$, the underlying curve, using a penalized smoothing method.

Penalized smoothing

Fitting a basis expansion is basically done with least squares:

$$S(\mathbf{c}_n) = \sum_j \left(Y_{jn} - \sum_k c_{nk} B_k(t_{nj}) \right)^2 .$$

A penalized approach penalizes the resulting function to promote different properties (such as smoothness):

$$S_\lambda(\mathbf{c}_n) = \sum_j \left(Y_{jn} - \sum_k c_{nk} B_k(t_{nj}) \right)^2 + \lambda \int_0^1 [L(\tilde{X}_n)(t)]^2 \, dt,$$

where we use $\tilde{X}_n(t) = \sum_k c_{nk} B_k(t_{nj})$ for notational convenience. L is some specified linear differential operator (usually second derivative).

Penalized smoothing - L

There is quite a bit of flexibility in choosing L. In general one can specify it as

$$L(\cdot) := \sum_{m=0}^{M} \alpha_m D^{(m)}(\cdot).$$

Common examples are first and second derivatives. A popular choice for periodic data is the harmonic acceleration operator

$$L(x)(t) = \frac{4\pi^2}{T^2} x^{(1)}(t) + x^{(3)}(t).$$

Penalized smoothing - Basis

The solution to the penalized regression equation can be written down in a closed form. Notice that

$$L(\tilde{X}_n)(t) = \sum_k c_{nk} L(B_k)(t) \Longrightarrow \int_0^1 [L(\tilde{X}_n)(t)]^2 = \mathbf{c}_n^\top \mathbf{W} \mathbf{c}_n,$$

where

$$W_{ij} = \int_0^1 L(B_i)(t) L(B_j)(t)\, dt.$$

Penalized smoothing - Basis

So, define the vector $\mathbf{Y}_n = \{Y_{nj}\}$ and matrix $\mathbf{B}_n = \{B_k(t_{nj})\}$, then the penalized regression equation can be expressed as

$$S(\mathbf{c}_n) = (\mathbf{Y}_n - \mathbf{B}_n\mathbf{c}_n)^\top(\mathbf{Y}_n - \mathbf{B}_n\mathbf{c}_n) + \lambda\mathbf{c}_n^\top\mathbf{W}\mathbf{c}_n.$$

This is just a ridge regression, so the solution is given by

$$\hat{\mathbf{c}}_n = (\mathbf{B}_n^\top\mathbf{B}_n + \lambda\mathbf{W})^{-1}\mathbf{B}_n^\top\mathbf{Y}_n.$$

Notice that if all curves are observed at same time points, then the $\mathbf{B}_n \equiv \mathbf{B}$. Once we have $\hat{\mathbf{c}}_n$ we can predict $\hat{X}_n(t)$ for any value of t. The fitted values are $\hat{\mathbf{Y}}_n = \mathbf{B}_n\hat{\mathbf{c}}_n$.

Penalized smoothing - Degrees of Freedom

To choose λ it helps to have the "degrees of freedom" from the model fit which is usually defined as

$$df = \text{trace}(\mathbf{B}_n(\mathbf{B}_n^\top \mathbf{B}_n + \lambda \mathbf{W})^{-1} \mathbf{B}_n^\top).$$

Notice that if $\lambda = 0$ then

$$df = \text{trace}((\mathbf{B}_n^\top \mathbf{B}_n)^{-1} \mathbf{B}_n^\top \mathbf{B}_n) = K.$$

Penalized smoothing - Choosing λ

To choose λ there are a number of ways. First, define

$$RSS = (\mathbf{Y}_n - \hat{\mathbf{Y}}_n)^\top (\mathbf{Y}_n - \hat{\mathbf{Y}}_n).$$

- $GCV(\lambda) = \frac{J}{(J-df)^2} RSS.$
- $AIC(\lambda) = J \log(J^{-1} RSS) + 2df$
- $BIC(\lambda) = J \log(J^{-1} RSS) + \log(J) df$
- Cross-validation

One would choose the λ which minimizes one of the above. GCV is maybe the most popular in FDA. Regardless, one must ALWAYS visually inspect the results to see if they make sense.

Penalized smoothing - Choosing λ

Consider a vector of outcomes, $\mathbf{Y} \in \mathbb{R}^N$, from some arbitrary model but whose predicted values can be expressed as

$$\hat{\mathbf{Y}} = \mathbf{H}\mathbf{Y},$$

where $\mathbf{H}$ is some matrix which does not depend on $\mathbf{Y}$. Then the GCV is defined as

$$GCV = \frac{N|\mathbf{Y} - \hat{\mathbf{Y}}|^2}{(N - \text{trace}(\mathbf{H}))^2},$$

this part of why it is so popular in FDA, very easy to compute for a variety of models.

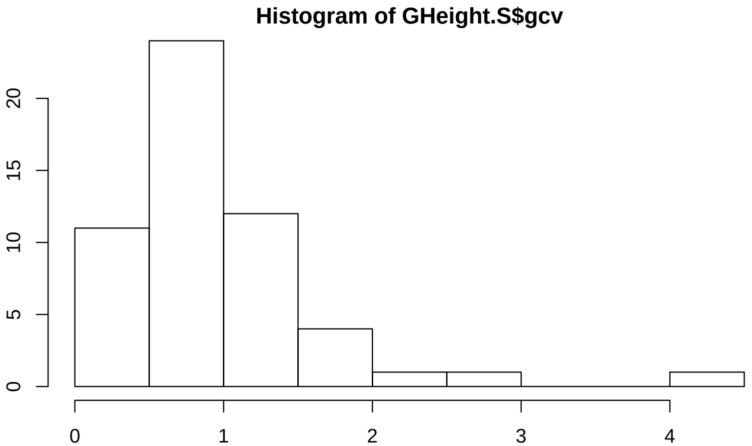
Penalized smoothing - R

We have been using `Data2fd` for function conversion, and it allows for smoothing, but it doesn't report the GCV. For more controlled smoothing we will use `smooth.basis`.

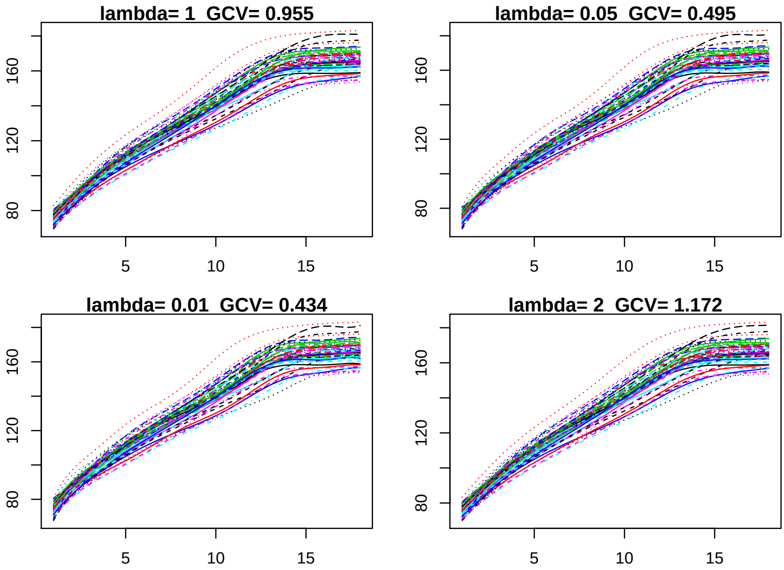
```
times = growth$age; GHeight = growth$hgtf
my_basis<-create.bspline.basis(c(1,18),
            nbasis=10,norder=5)
my_par<-fdPar(my_basis,Lfdobj=2,lambda=1)
GHeight.S<-smooth.basis(times,GHeight,my_par)
names(GHeight.S)[1:5]; names(GHeight.S)[6:9]

## [1] "fd"    "df"    "gcv"   "beta" "SSE"
## [1] "penmat"  "y2cMap"  "argvals" "y"
```

Penalized smoothing - R

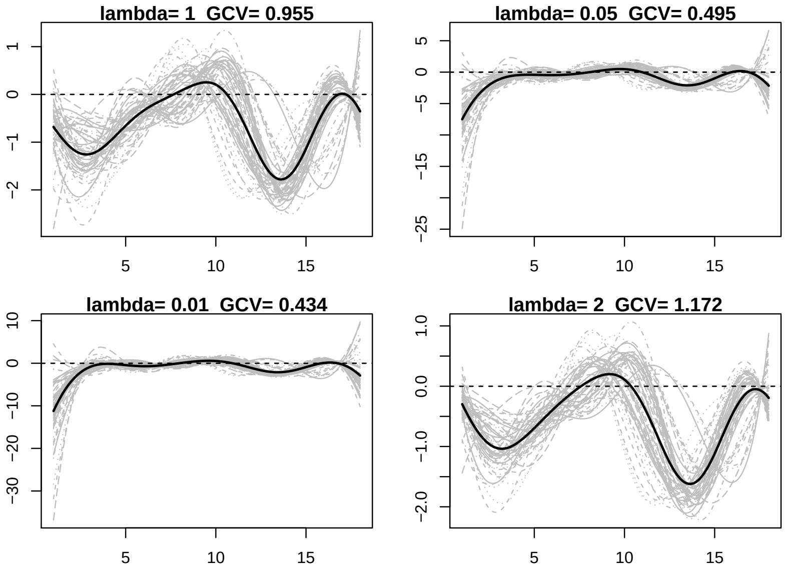
```
mean(GHeight.S$gcv)

## [1] 0.9545315

hist(GHeight.S$gcv)
```



Penalized smoothing - R



Berkeley - 2nd Derivatives



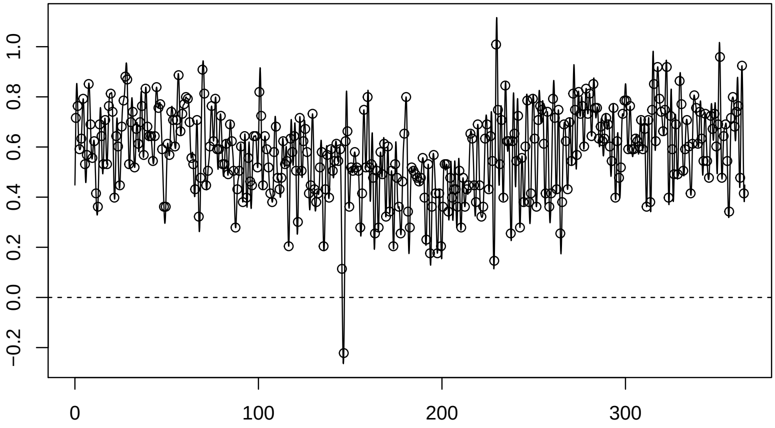
Example - Canadian Weather

The `CanadianWeather` data is also part of the `fda` package. It consists of daily temperature and precipitation data at 35 locations in Canada. Each daily measurement is an average across the years 1960 to 1994, so each station produces only one curve.

```
nbasis = 365; yearRng = c(0,365)
daybasis = create.fourier.basis(yearRng, nbasis)
logprecav = CanadianWeather$dailyAv[,,'log10precip']
dayprecfd <- with(CanadianWeather, smooth.basis(day.5,
        logprecav, daybasis,
        fdnames=list("Day","Station","log10(mm)"))$fd)
names(CanadianWeather)[1:3];names(CanadianWeather)[4:6];nam

## [1] "dailyAv"  "place"    "province"
## [1] "coordinates" "region"      "monthlyTemp"
## [1] "monthlyPrecip" "geogindex"
```

Example - Canadian Weather

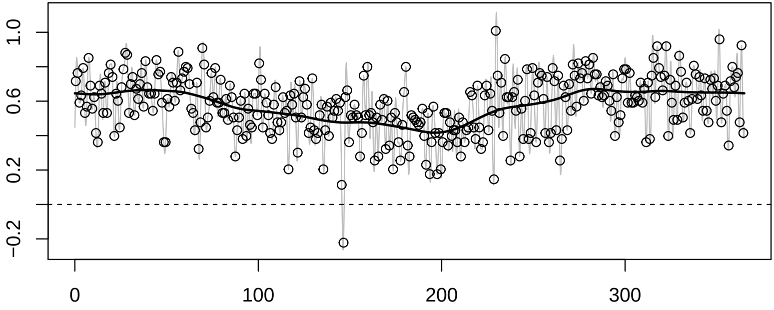
```
par(mar=c(3,3,1,1))
plot(dayprecfd[1]);points(day.5,logprecav[,1])
```



Example - Canadian Weather

Lets smooth it up some

```
par(mar=c(3,3,1,1))
daybasis = create.fourier.basis(yearRng, nbasis)
mypar = fdPar(daybasis,Lfdobj=2,lambda=10000)
Y.f<-smooth.basis(day.5,logprecav,mypar)
plot(dayprecfd[1],col='grey');points(day.5,logprecav[,1])
plot(Y.f$fd[1],add=TRUE,lwd=2)
```



Example - Canadian Weather

```
mypar = fdPar(daybasis,Lfdobj=2,lambda=.001)
Y.f2<-smooth.basis(day.5,logprecav,mypar)
mean(Y.f2$gcv)

## [1] 0.08145941

mean(Y.f$gcv)

## [1] 0.04038778
```