Functional Data Analysis (Lecture 3) – FDA package: smoothing

Zoltán Szabó

October 18, 2016

Reminder

- Create, evaluate, plot basis systems: $\{\phi_k\}_{k=1}^{B}$,
- in FDA toolbox: basis object.

Basis system with coefficients: $\{\phi_k\}_{k=1}^{B}, \mathbf{c}$

Functional data (fd) object

Create:

```
>>basis_Fourier  = create_fourier_basis([0,2*pi],5);
>>coeffs = rand(5,2); %coefficients
  %B x N x m; B = |basis|, N = |repetitions|, m = dim(x_i)
>>fd_Fourier = fd(coeffs,basis_Fourier);
>>plot(fd_Fourier);
```

Labels to an fd object: fdnames object

```
>>fdnames_Fourier = cell(1,3);
>>fdnames_Fourier{1} = 'Time (t)';
>>fdnames_Fourier{2} = ['Trial1'; 'Trial2'];
>>fdnames_Fourier{3} = 'Approximation (y)';
>>fd_Fourier = fd(coeffs,basis_Fourier,fdnames_Fourier);
>>plot(fd_Fourier);
```

Evaluate fd object, its derivatives; Lfd object

```
>>tvec = linspace(0,pi,20);
>>xhat = eval_fd(tvec,fd_Fourier);
>>figure; plot(tvec,xhat);

>>xhat_D = eval_fd(tvec,fd_Fourier,1);
>>figure; plot(tvec,xhat_D);

%linear differential operators (Lfd object):
>>Lfd_D2 = int2Lfd(2); %L=D^2:
>>xhat_D2 = eval_fd(tvec,fd_Fourier,Lfd_D2);
>>figure; plot(tvec,xhat_D2);

>>omega=1; Lfd_harmonic = vec2Lfd([0,omega^2,0],[0,2*pi]);
>>xhat_harmonic = eval_fd(tvec,fd_Fourier,Lfd_harmonic);
>>figure; plot(tvec,xhat_harmonic);
```

Possible (see `help Lfd`): $Lx(t) = \sum_{j=0}^{r} \beta_j(t) D^j x(t)$.

Objective function: fdPar object

$L = D^m$:

```
>>fdPar_my = fdPar(basis_or_fd_my,m_my,lambda_my);
```

General L:

```
>>fdPar_my = fdPar(basis_or_fd_my,L_my,lambda_my);
```

Smoothing

Berkeley growth dataset

Dataset description:

- heights of 54 subjects,
- measurements (31) for age=$1-18$.

Load data:

```
>>N = 54; %# of subjects
>>n = 31; %# of measurements for each subject
>>fid = fopen('hgtf.dat','rt');
>>height = reshape(fscanf(fid,'%f'),[n,N]);
>>fclose(fid);
>>age = [1:0.25:2, 3:8, 8.5:0.5:18]';
```

Plan

Smoothing with

1. least squares (small B).
2. regularization (L, λ).
3. regularization (L, $\hat{\lambda}$): $\hat{\lambda} = \arg\min_{\lambda} GCV(\lambda)$.

Smoothing with least squares

Create spline basis ($B = 12$):

```
>>rng_age = [1,18];
>>m = 6;
>>B = 12; %massive regularization: B < 35
>>basis_spline12 = create_bspline_basis(rng_age,B,m);
                   %uniformly placed knots
```

Smooth the data, plot:

```
>>fd_smoothed12 = smooth_basis(age,height,basis_spline12);
>>plotfit_fd(height,age,fd_smoothed12); %use the arrows!
```

Note: basis was used as fdPar; it makes sense (no λ, L).

Smoothing with regularization ($L = D^4$, $\lambda = 0.1$)

Create spline basis:

```
>>rng_age = [1,18];
>>knots = age;
>>m = 6; %order
>>B = length(knots) + m - 2; %# of basis functions
>>basis_spline = create_bspline_basis(rng_age,B,m,knots);
```

Regularization:

```
>>Lfd_spline  = int2Lfd(4); %L=D^4
>>lambda = 1/10; %regularization parameter
>>fdPar_spline = fdPar(basis_spline,Lfd_spline,lambda);
```

Smooth the data, plot:

```
>>fd_smoothed = smooth_basis(age,height,fdPar_spline);
>>plotfit_fd(height,age,fd_smoothed); %use the arrows!
```

Smoothing with regularization: $\hat{\lambda} = \arg\min_\lambda GCV(\lambda)$

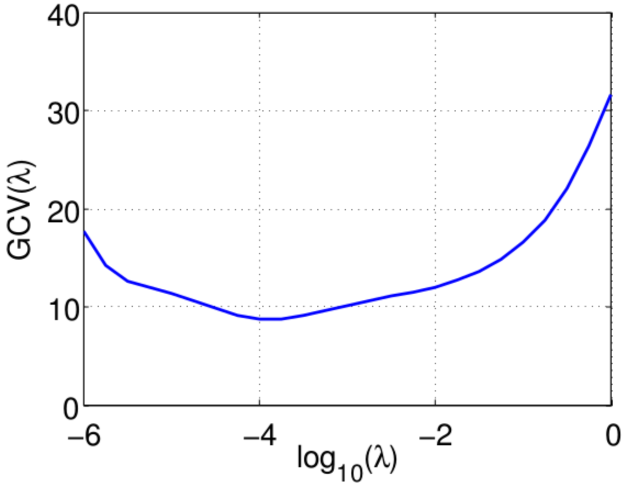
Load data, create spline basis and L: done. The rest:

```
>>log10lam   = [-6:0.25:0];
>>gcv_save = zeros(length(log10lam),1);
>>for i = 1 : length(log10lam)
>> fdPar_i = fdPar(basis_spline, Lfd_spline, 10^log10lam(i));
>> [fd_smoothed_i,df_i,gcv_i]=smooth_basis(age,height,fdPar_i);
>> gcv_save(i) = sum(gcv_i); %multiple subjects
>>end
```

Plot:

```
>>plot(log10lam, gcv_save);
>>xlabel('log_{10}(\lambda)');
>>ylabel('GCV(\lambda)');
```

Smoothing with regularization: $\log_{10}(\lambda) \mapsto GCV(\lambda)$



Estimation: $\hat{\lambda} \approx 10^{-4}$.

Smoothing with constraints

Monotone smoothing

$$x(t) = \beta_0 + \beta_1 \int_{t_0}^{t} e^{W(u)} du.$$

- Relevant function: `smooth_monotone`.
- Other constraints:
  1. positivity: `smooth_pos`,
  2. pdf: `density_fd`.

Berkeley growth data: monotone smoothing

load data:

```
>>N = 54; n = 31;
>>fid = fopen('hgtf.dat','rt');
>>height = reshape(fscanf(fid,'%f'),[n,N]);
>>fclose(fid);
>>age = [1:0.25:2, 3:8, 8.5:0.5:18]'; %n = |age|
```

basis, L, λ:

```
>>rng_age = [1,18]; m = 6; B = length(age) + m - 2;
>>basis_spline = create_bspline_basis(rng_age,B,m,age);
>>fd_spline = fd(zeros(B,N),basis_spline);      %J + init.
>>fdPar_spline = fdPar(fd_spline,3,10^(-0.5)); %L=D^3
```

monotone smoothing:

```
[W_hat,beta_hat,height_hat] =
                smooth_monotone(age,height,fdPar_spline);
```

Summary

Objects:

- fd: $\mathbf{c}^T\phi$.
- fdnames: labels for fd.
- Lfd: linear differential operator (L).
- fdPar: objective function (J).

We covered Chapter 4-5 in [2].