Functional Data Analysis (Lecture 5) - Functional PCA

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November 15, 2016

One-page summary

- Last time:
  - PCA,
  - linear dimensionality reduction in $\mathbb{R}^d$,
  - principle of maximum variance, minimal approximation error.

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  - principle of maximum variance, minimal approximation error.
- Today:
  1. functional extension of PCA.

Functional PCA

fPCA: Keywords

- Preprocessing steps: smoothing, curve registration.
- Goal:
  - find a low-dimensional subspace of curves,
  - capturing the characteristic patterns.

PCA

- Given: $X = \{\mathbf{x}_i\}_{i=1}^N \subset \mathbb{R}^D$.
- Preprocessing: centering, i.e. $\mathbf{x}_i \to \mathbf{x}_i - \mathbb{E}\mathbf{x}$.

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- Objective: maximize the variance of the projection

$$\max_{\mathbf{w}\in\mathbb{R}^D:\|\mathbf{w}\|_2=1} \mathbf{w}^T\boldsymbol{\Sigma}\mathbf{w}, \text{ where } \boldsymbol{\Sigma} = \frac{1}{N}\sum_{i=1}^N \mathbf{x}_i\mathbf{x}_i^T.$$

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- Solution: $\boldsymbol{\Sigma}\mathbf{w} = \lambda\mathbf{w}$, top d-eigenvectors.

PCA vs. fPCA

Covariance function:

$$v_{s,t} = \frac{1}{N}\sum_{i=1}^{N}(\mathbf{x}_i)_s(\mathbf{x}_i)_t \qquad v(s,t) = \frac{1}{N}\sum_{i=1}^{N}x_i(s)x_i(t).$$

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Covariance operator ($\boldsymbol{\Sigma} = [v(s,t)]_{s,t}$):

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$$\|\mathbf{w}\|_2 = \sqrt{\sum_i w_i^2} = 1, \qquad \|w\|_{L^2} = \sqrt{\int w^2(t)dt} = 1.$$

fPCA: Different, equivalent views

1. Find $W = \{w_i\}_{i=1}^d$ ONS in L^2 minimizing

$$\mathbb{E}_x \|x - \hat{x}\|_{L^2}, \qquad \hat{x} = \sum_{i=1}^d \langle w_i, x \rangle_{L^2} w_i.$$

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$$\Sigma w = \lambda w, \qquad \Sigma = [v(s,t)], \qquad v(s,t) = \frac{1}{N}\sum_{i=1}^N x_i(s)x_i(t).$$

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Challenge

How do we solve the $\Sigma w = \lambda w$ eigenproblem?

Solution-1: Discretizing the functions

1. Discretize x_i-s at a fine grid: $\{s_j\}_{j=1}^n$, $h := |s_j - s_k|$.
2. $X := [x_i(s_j)]_{i=1,\ldots,N;j=1,\ldots,n} \in \mathbb{R}^{N\times n}$.

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3. Solve the standard eigensystem: $\boldsymbol{\Sigma}\mathbf{w} = \lambda\mathbf{w}$, $\boldsymbol{\Sigma} = \frac{X^T X}{N}$
   $\Rightarrow \hat{\mathbf{w}} = [w(s_j)] \in \mathbb{R}^n$.

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Solution-2: Basis function expansion

- Idea: solve $\Sigma w = \lambda w$ in *span* $(\phi_1, \ldots, \phi_B)$.

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- Idea: solve $\Sigma w = \lambda w$ in $span\left(\phi_1, \ldots, \phi_B\right)$.
- Assume

$$x_i = \langle \mathbf{c}_i, \phi(t) \rangle, \text{ i.e., } \qquad x_i(t) = \sum_{k=1}^{B} c_{ik}\phi_k(t),$$

$$w(s) = \langle \mathbf{b}, \phi(s) \rangle, \qquad w(s) = \sum_{k=1}^{B} b_k\phi_k(s).$$

Solution-2: Basis function expansion – continued

- Assumption: $x_i = \langle \mathbf{c}_i, \phi(t) \rangle$, $w(s) = \langle \mathbf{b}, \phi(s) \rangle$. Then

$$\mathbf{x}(t) = [x_1(t); \ldots; x_N(t)] = \mathbf{C}\phi(t), \quad (\mathbf{C} \in \mathbb{R}^{N \times B}),$$

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- Thus, $(\Sigma w)(s) = \lambda w(s)$ takes the form:

$$\frac{1}{N}\phi^T(s)\mathbf{C}^T\mathbf{CWb} = \lambda\phi^T(s)\mathbf{b}, \quad \forall s.$$

Solution-2: Basis function expansion – continued

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In practise one solves the symmetric eigenvalue task $[\mathbf{W}^{\frac{1}{2}} \times (1)]$:

$$\frac{1}{N}\mathbf{W}^{\frac{1}{2}}\mathbf{C}^T\mathbf{C}\mathbf{W}^{\frac{1}{2}}\underbrace{\mathbf{W}^{\frac{1}{2}}\mathbf{b}}_{=:\mathbf{u}} = \lambda\mathbf{W}^{\frac{1}{2}}\mathbf{b},$$

and takes $\mathbf{b} = \mathbf{W}^{-\frac{1}{2}}\mathbf{u}$ for the $\mathbf{u}$ eigenvectors.

Solution-2: notes/specific cases

Recall: $\frac{1}{N}\mathbf{W}^{\frac{1}{2}}\mathbf{C}^T\mathbf{C}\mathbf{W}^{\frac{1}{2}}\mathbf{W}^{\frac{1}{2}}\mathbf{b} = \lambda\mathbf{W}^{\frac{1}{2}}\mathbf{b}$. If

1. $\mathbf{W} = \mathbf{I}$, i.e. $\{\phi_k\}_{k=1}^B$ is an ONS $\Rightarrow$ standard

   eigenanalysis of $\frac{\mathbf{C}^T\mathbf{C}}{N}$.

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2. Other extreme: $\phi_i := x_i$ $(\forall i) \Rightarrow \mathbf{C} = \mathbf{I}$,

   eigenanalysis of $\frac{\mathbf{W}}{N}$,

   where $\mathbf{W} = [W_{ij}]$, $W_{ij} = \int x_i(t)x_j(t)dt \leftarrow$ quadrature methods.

Extensions-1: Better discretization strategies

- Recall: $\int v(s_j, t)w(t)dt \approx h \sum_{k=1}^{n} v(s_j, s_k)w(s_k)$, $\forall s_j$.

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1. n: number of quadrature points.
2. h_j: quadrature weights (previously: $h_j = h$, $\forall j$).
3. s_j: quadrature points.

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Smart choice of locations (s_j) and weights (h_j) can help!

Extensions-1: Better discretization

In this case: $\Sigma w \approx \mathbf{\Sigma H w}$, $\mathbf{w} := [w(s_j)]$, $\mathbf{H} := diag(h_j)$. Thus

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Symmetric form $[\mathbf{H}^{\frac{1}{2}} \times (2)]$:

$$\mathbf{H}^{\frac{1}{2}} \mathbf{\Sigma} \mathbf{H}^{\frac{1}{2}} \underbrace{\mathbf{H}^{\frac{1}{2}} \mathbf{w}}_{=:\mathbf{u}} = \lambda \mathbf{H}^{\frac{1}{2}} \mathbf{w}. \tag{3}$$

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Recipe:

1. Solve (3) for $\mathbf{u}$, compute $\mathbf{w} = \mathbf{H}^{-\frac{1}{2}} \mathbf{u}$.
2. Optional: apply interpolation on $\{(\mathbf{w})_j = w(s_j)\}_{j=1}^{n}$.

Extensions-2

- Until now: $x_i(t) \in \mathbb{R}$.
- In practice:
  - $x_i(t) \in \mathbb{R}^L$ can be useful.
  - Example: handwriting, joint moving of body parts, ...

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- In practice:
  - $x_i(t) \in \mathbb{R}^L$ can be useful.
  - Example: handwriting, joint moving of body parts, ...
- With a (re-) definition of the inner product:

$$\langle \mathbf{u}(t), \mathbf{v}(t) \rangle := \sum_{\ell=1}^{L} \langle u_\ell, v_\ell \rangle = \sum_{\ell=1}^{L} \int u_\ell(t) v_\ell(t) dt$$

one can do fPCA similarly.

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  2. Vector-valued functions: inner product overloading.

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  1. Discretization.
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We covered the 'functional part' of Chapter 8 in [1].