Functional Data Analysis (Lecture 6) - Regularized functional PCA

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One-page summary

- Last time:
  - functional PCA (=:fPCA),
  - $var_x \langle w, x \rangle \to \max_{w:\|w\|_2=1}$.

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- Today:
  - regularized fPCA.

Regularized fPCA

Regularized fPCA: objective

- Idea: modify the fPCA objective with a smoothness term.
- Old objective:

$$J_0(w) = var_x \langle w, x \rangle \to \max_{w:\|w\|_2=1}.$$

- New objective ($\lambda > 0$):

$$J(w) = \frac{var_x \langle w, x \rangle}{\|w\|^2 + \lambda PEN_2(w)} \to \max_w,$$

$$PEN_2(w) = \left\|D^2 w\right\|^2.$$

Regularized fPCA

- Idea: Apply basis function expansion.
- Assumption:

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$$var_x \langle w, x \rangle = \frac{1}{n} \sum_{i=1}^{n} \left(\mathbf{b}^T \mathbf{J} \mathbf{c}_i \right) \left(\mathbf{c}_i^T \mathbf{J} \mathbf{b} \right)$$

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$$\begin{aligned} \langle w, x_i \rangle &= \int w(t) x_i(t) dt = \int \mathbf{b}^T \phi(t) \phi^T(t) \mathbf{c}_i dt \\ &= \mathbf{b}^T \underbrace{\left[\int \phi(t) \phi^T(t) dt \right]}_{=:\mathbf{J}} \mathbf{c}_i, \end{aligned}$$

$$var_x \langle w, x \rangle = \frac{1}{n} \sum_{i=1}^{n} \left(\mathbf{b}^T \mathbf{J} \mathbf{c}_i \right) \left(\mathbf{c}_i^T \mathbf{J} \mathbf{b} \right) = \mathbf{b}^T \mathbf{J} \underbrace{\left(\frac{1}{n} \sum_{i=1}^{n} \mathbf{c}_i \mathbf{c}_i^T \right)}_{=:\mathbf{V}} \mathbf{J} \mathbf{b}.$$

Regularized fPCA: denominator

Using

$$w(t) = \mathbf{b}^T \phi(t) = \sum_j b_j \phi_j(t),$$

one gets

$$\|w\|^2 = \int \mathbf{b}^T \phi(t) \phi(t)^T \mathbf{b} dt$$

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Regularized fPCA: collect the terms

Until now:

$$
\begin{aligned}
var \langle w, x \rangle &= \mathbf{b}^T \mathbf{J} \mathbf{V} \mathbf{J} \mathbf{b}, \\
\|w\|^2 &= \mathbf{b}^T \mathbf{J} \mathbf{b}, \\
PEN_2(w) &= \mathbf{b}^T \mathbf{K} \mathbf{b}.
\end{aligned}
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Regularized fPCA: collect the terms

Until now:

$$\begin{aligned} var\left\langle w, x\right\rangle &= \mathbf{b}^T\mathbf{JVJb}, \\ \left\|w\right\|^2 &= \mathbf{b}^T\mathbf{Jb}, \\ PEN_2(w) &= \mathbf{b}^T\mathbf{Kb}. \end{aligned}$$

Thus

$$J(w) = \frac{var_x\left\langle w, x\right\rangle}{\left\|w\right\|^2 + \lambda PEN_2(w)} = \frac{\mathbf{b}^T\mathbf{JVJb}}{\mathbf{b}^T\mathbf{Jb} + \lambda\mathbf{b}^T\mathbf{Kb}}.$$

Regularized fPCA: final eigenproblem

The objective function:

$$J(w) = \frac{\mathbf{b}^T \mathbf{JVJb}}{\mathbf{b}^T \mathbf{Jb} + \lambda \mathbf{b}^T \mathbf{Kb}},$$

which is equivalent to the eigenproblem

$$\mathbf{JVJb} = \lambda(\mathbf{J} + \lambda \mathbf{K})\mathbf{b}.$$

Regularized fPCA: Fourier basis

In case of Fourier basis simplifications happen.

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\begin{aligned}
\mathbf{J} &= [\langle \phi_i, \phi_j \rangle] = [\delta_{ij}] = \mathbf{I}, \\
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Here, with $\phi_{2j-1}(t) = \sin(2\pi j t)$, $\phi_{2j}(t) = \cos(2\pi j t)$, $a_{2j-1} := a_{2j} = 2\pi j$

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λ-estimation

For fixed smoothing parameter (λ):

- $\{x_i\}_{i=1}^n \backslash \{x_i\} \rightarrow$ eigenfunctions: $\{w_j^i(\lambda)\}_{j=1}^d$.

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$$CV_d(\lambda) = \sum_{i=1}^n \left\| e_d^i(\lambda) \right\|^2.$$

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- d-independent cross-validation ($d \leqslant n-1$):

$$CV(\lambda) = \sum_d CV_d(\lambda).$$

Summary

- Functional PCA (pca_fd).
- Old objective + smoothing term (λ),
- Eigenvalue problem.
- λ choice: cross-validation.

We covered Chapter 9 in [1], 'fPCA part' of Chapter 7 in [2].