Scalar on Function Regression

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Presentation Day

Introduction

- Near-infrared (NIR) spectroscopy enables fast diagnostics by using the NIR region of the electromagnetic spectrum
- Suited for field-monitoring / on-line analysis and diagnostics of e.g: prediction of octane ratings!
- Spectroscopy results in high-dimensional dataset.
- This set of measurements along a continuum can be viewed as set of smooth spectral curves
- Regression to determine relationship between octane rating and spectral curves

Theory

- A simple functional dataset is given by $x_n(t_{j,n}) \in \mathbb{R}, t_{j,n} \in [T_1, T_2], n = 1, 2, ..., N, j = 1, 2, ..., J_n$
- Continuous underlying process, where $x_n(t)$ exists at any point t, but is only observed at $x_n(t_{j,n})$, eg.: growth curves, financial data, human perception (music pitch,...).
- To abstract information from the curves, they must be interpretable!

Theory

Jonghun

- Random Functions (name square integrable functions)
- Motivate continuous stochastic processes (growth curves/electricity consumption/yield curves/stonks)
- Use curves to predict a scalar response (show typical dgp)

Theory

Jonghun

- Basis expansions (b-splines and fourier)
- Talk about purposes
- Plots and show bias variance tradeoff

Theory

Jakob

- Random function represented as linear combination of basis functions ✓
- Just transform to multiple linear regression setting ✓
- You already know that from the beginning ✓

Estimation via Basis Representation

Assume the following data generating process

$$Y(\omega) = \alpha + \int_0^1 \beta(s)F(\omega)(s)\mathrm{d}s + \epsilon(\omega)$$

- Y and ϵ realize in $\mathbb{R}$ and F realizes in $\mathbb{L}^2[0,1]$

Assume that we have a data set containing observations each of which is made up of:

- y_i: a scalar realization of Y
- $f_i(t)$: a realization of F

Estimation via Basis Representation

Let $\{b_i(t) \mid i = 1, \ldots, \infty\}$ be a basis of $\mathbb{L}^2[0,1]$

Then we have the following representation of $\beta(t)$

$$\beta(t) = \sum_{j=1}^{\infty} \psi_j b_j(t) = \sum_{j=1}^{L} \psi_j b_j(t) + \delta(t) \approx \sum_{j=1}^{L} \psi_j b_j(t)$$

and we can transform the data generating process into:

$$\begin{aligned} Y(\omega) &= \alpha + \int_0^1 \left[\left(\sum_{j=1}^{\infty} \psi_j b_j(s) \right) F(\omega)(s) \right] \mathrm{d}s + \epsilon(\omega) \\ &= \alpha + \sum_{j=1}^{\infty} \left[\psi_j \int_0^1 F(\omega)(s) b_j(s) \mathrm{d}s \right] + \epsilon(\omega) \end{aligned}$$

Estimation via Basis Representation

$$Z_j(\omega) = \int_0^1 F(\omega)(s) b_j(s) \mathrm{d}s$$

This is a scalar random variable leading to the following transformation

$$Y(\omega) = \alpha + \sum_{j=1}^{\infty} \psi_j Z_j(\omega) + \epsilon(\omega)$$

Each combination of observation $f_i(t)$ and deterministic basis function $b_j(t)$ effectively gives us a realization of this random variable.

$$Z_{i,j} = \int_0^1 f_i(s) b_j(s) \mathrm{d}s$$

Estimation via Basis Representation

This allows us to write each observation in the data set as

- y_i: a scalar realization of Y
- $(Z_{i,j})_{j \in \mathbb{N}}$: a countably infinite sequence of scalars

Truncating the functional basis allows us to approximate the data set in the usual multivariate form.

- y_i: a scalar realization of Y
- $(Z_{i,1} \ \ldots \ Z_{i,L})'$: a vector of scalar regressors

Coefficients can then be estimated using theory from multivariate regression leading to an estimated coefficient vector $\hat{\psi}_L \in \mathbb{R}^L$.

Estimation via Basis Representation

This can be translated into an estimated coefficient function $\hat{\beta}(t)$:

$$\hat{\beta}_L(t) = \sum_{j=1}^{L} \hat{\psi}_{L,j} b_j(t)$$

This is dependent on...

- The functional basis $(b_j(t))_{j \in \mathcal{I}}$ for the estimation of $\beta(t)$
- The truncation parameter L
- (The functional basis used to approximate the observations)
- (The truncation parameter in the approximation of the observations)

Theory - FPCA

Jakob

- Let's assume you know the theory of PCA (pc from varcov matrix) ✓
- Introduce mean and covariance functions of random functions ✓
- There is another cool basis $\rightarrow$ Eigenbasis (Karhunen-Loeve Expansion) ✓
- Sample Analog! (create a basis from observations and use for basis regression) ✓
- Plot fpcs and approximation of function realization

Spectral Representation of Random Vectors

Let $X(\omega)$ be a random vector realizing in $\mathbb{R}^p$.

- Let $\mu_x = \mathbb{E}(X)$ and $\Sigma_X = Cov(X)$
- Let $\{\gamma_i \mid i = 1, \ldots, p\}$ be the orthonormal **Eigenvectors** of Σ_X
- Let $\{\lambda_i \mid i = 1, \ldots, p\}$ be the corresponding **Eigenvalues** of Σ_X

Then X can also be represented as

$$X(\omega) = \mu_x + \sum_{i=1}^{p} \xi_i(\omega)\gamma_i$$

where the $\xi_i(\omega)$ have the following properties

1. $\mathbb{E}[\xi_i(\omega)] = 0$
2. $Var(\xi_i(\omega)) = \lambda_i$
3. $Cov(\xi_i(\omega), \xi_j(\omega)) = 0$ for $i \neq j$

Karhunen-Loéve Expansion

Mean Function:

$$\mu(t) = \mathbb{E}\left[F(\omega)(t)\right]$$

Autocovariance Function:

$$c(t,s) = \mathbb{E}\Big[\left(F(\omega)(t) - \mu(t)\right)\left(F(\omega)(s) - \mu(s)\right)\Big]$$

The **Eigenvalues** and **Eigenfunctions**: $\{(\lambda_i, \nu_i) \mid i \in \mathcal{I}\}$ are solutions of the following equation:

$$\int_0^1 c(t,s)\nu(s)\mathrm{d}s = \lambda\nu(t)$$

Karhunen-Loéve Expansion

A random function F can be expressed in terms of its mean function and its Eigenfunctions:

$$F(\omega)(t) = \mu(t) + \sum_{j=1}^{\infty} \xi_j(\omega)\nu_j(t)$$

Where the ξ_j are scalar-valued random variables with the following properties.

1. $\mathbb{E}[\xi_i(\omega)] = 0$
2. $Var(\xi_i(\omega)) = \lambda_i$
3. $Cov(\xi_i(\omega), \xi_j(\omega)) = 0$ for $i \neq j$

This representation is called the **Karhunen-Loéve Expansion** of the random function F and the Eigenfunctions can serve as a basis to represent the function.

Principal Component Analysis

A related concept is **Principal Component Analysis** (PCA).

Σ_X unknown $\rightarrow$ **sample analogues**

- Let $\mathbf{X} \in \mathbb{R}^{n \times p}$ contain the standardized regressors
- Let $\hat{\Sigma}_X = \frac{\mathbf{X}'\mathbf{X}}{n}$
- Let $\{\hat{\gamma}_i \mid i = 1, \ldots, p\}$ be the orthonormal **Eigenvectors** of $\hat{\Sigma}_X$
- Let $\{\hat{\lambda}_i \mid i = 1, \ldots, p\}$ be the corresponding **Eigenvalues** of $\hat{\Sigma}_X$

Then $Z_i(\omega) = \hat{\gamma}_i' X(\omega)$ is called the i'th principal component and

1. $\mathbb{E}[Z_i(\omega)] = 0$
2. $Var(Z_i(\omega)) = \hat{\lambda}_i$
3. $Cov(Z_i(\omega), Z_j(\omega)) = 0$ for $i \neq j$

Functional Principal Component Analysis

This idea can be extended to functional regressors in the form of **Functional Principal Component Analysis** (FPCA).

Empirical Mean Function:

$$\hat{\mu}(t) = \frac{1}{n} \sum_{j=1}^{n} f_j(t)$$

Empirical Autocovariance Function:

$$\hat{c}(t,s) = \frac{1}{n} \sum_{j=1}^{n} \left(f_j(t) - \hat{\mu}(t)\right) \left(f_j(s) - \hat{\mu}(s)\right)$$

Functional Principal Component Analysis

The **Eigenvalues** and **Eigenfunctions**: $\{(\hat{\lambda}_i, \hat{\nu}_i) \mid i \in \mathcal{I}\}$ are solutions of the following equation:

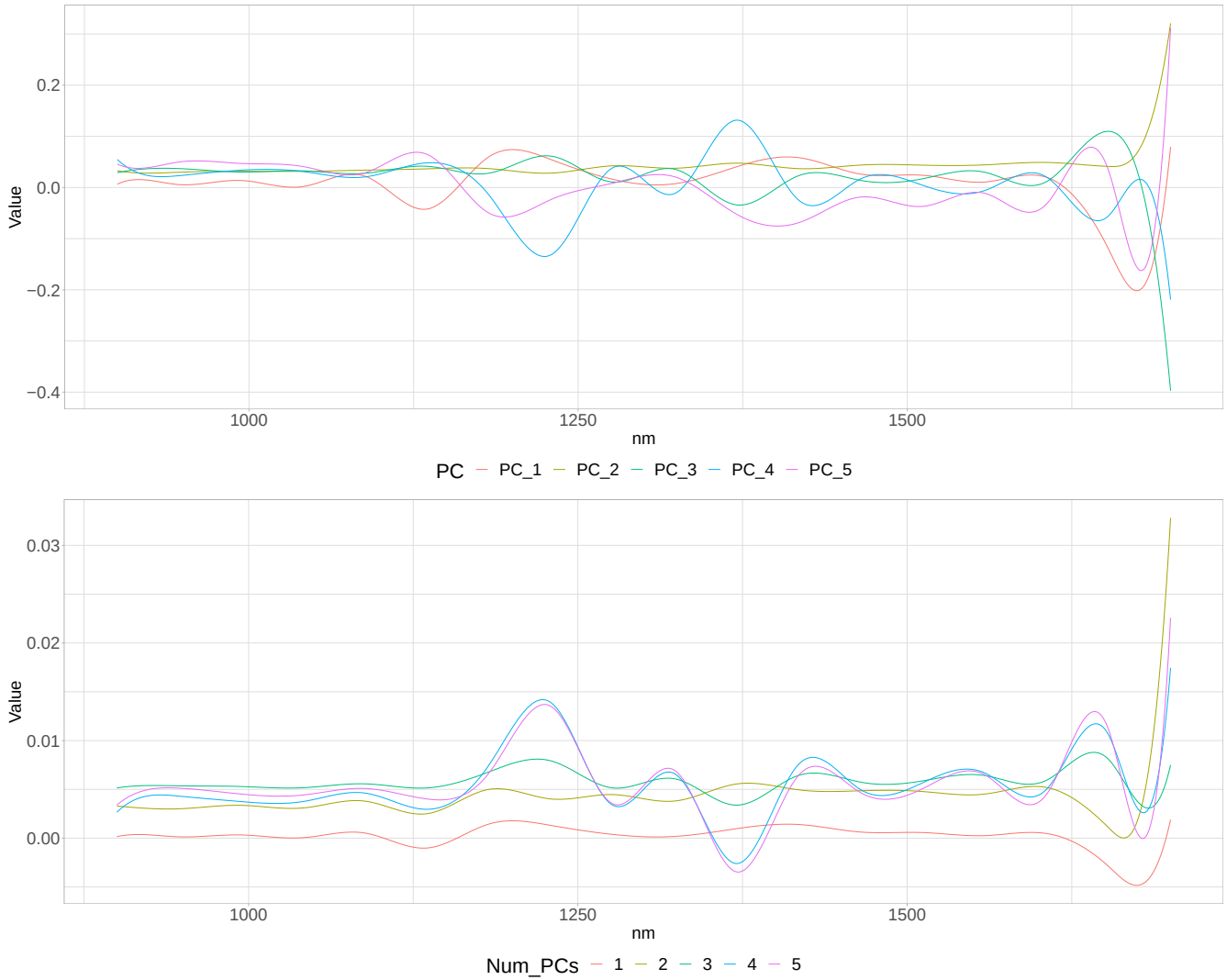
$$\int_0^1 \hat{c}(t,s)\hat{\nu}(s)\mathrm{d}s = \hat{\lambda}\hat{\nu}(t)$$

The $\{\hat{\nu}_i(s) \mid i \in \mathcal{I}\}$ are called **Functional Principal Components** and can serve as a basis for representing the original curves.

The corresponding scores $\hat{\xi}_i$ can be derived as

$$\hat{\xi}_j(\omega) = \int_0^1 (F(\omega)(s) - \hat{\mu}(s))\hat{\nu}_j(s)\mathrm{d}s$$

FPCA - Plots



Lorem Ipsum
Dolor Sit
Amet

Simulation Setup & Application

- Use the gasoline dataset (NIR-spectroscopy, 60×401) to predict octane ratings.
- Generate new curves from gasoline dataset, motivated by Karhunen-Loeve expansion:

$$F^{new}(\omega)(t) = \mu^{NIR}(t) + \sum_{j=1}^{\infty} \xi_j^{new} \nu_j(t)^{new}$$

where

$$\xi_j^{new} \in \mathcal{N}_n(0, \Sigma)$$

and $\nu_j(t)^{new}$ be a $grid \times n_{FPC}$ matrix.

Simulation Setup & Application cont.

- Following Reiss and Ogden (2007), let f_1 and f_2 be two true coefficient functions that differ in smoothness:

$$f_1 = 2\sin(0.5\pi t) + 4\sin(1.5\pi t) + 5\sin(2.5\pi t)$$

$$f_2 = 1.5^{\frac{-0,5(t-0.3)^2}{0.02^2}} - 4^{\frac{-0,5(t-0.45)^2}{0.015^2}} + 8^{\frac{-0,5(t-0.6)^2}{0.02^2}} - 1^{\frac{-0,5(t-0.8)^2}{0.03^2}}$$

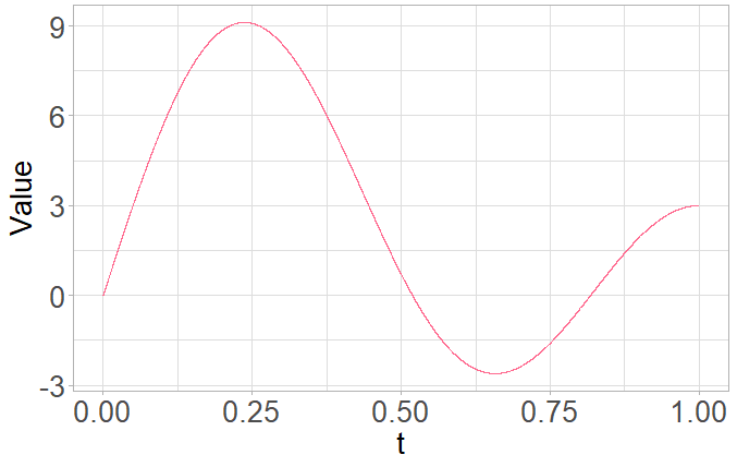


Figure: f_1, smooth function

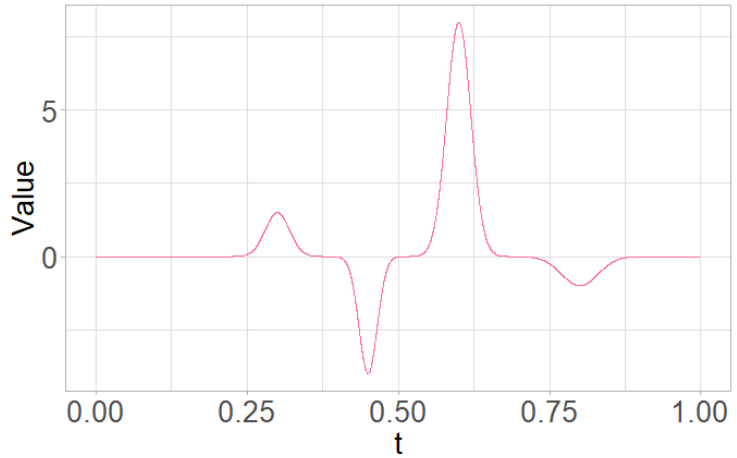


Figure: f_2, bumpy function

Simulation Setup & Application cont.

- Let

  $Y_{1,f} = \mathbf{NIR} \times \mathbf{f} + \mathcal{N}(0,1) \times var(NIR \times f)/0.9 - var(NIR \times f)$,
  $Y_{2,f} = \mathbf{NIR} \times \mathbf{f} + \mathcal{N}(0,1) \times var(NIR \times f)/0.9 - var(NIR \times f)$
  be two responses for $f \in f_1, f_2$.
- Four combinations with different number of cubic basis-function $n_{basis} \in (5, 6, ..., 25)$ to perform regression using basis expansion and the FPCR approach.
- Compare results via criteria (CV, Mallows CP,...)
- add results here!

Simulation Setup & Application cont.

- Use insights from the simulation study to uncover dependence.
- Similar setup, but using only bsplie basis expansion and initial 60 spectral curves.
- Validation set approach: Scores of testdata needs to be estimated by the trainingdata. explain in detail?
- Report results by MSE scaled by variance.

Summary

Jona

Just summarize what we have done...

further reading

Put footnotes here!