# Scalar on Function Regression

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Presentation Day

# Introduction

Jona
Introductory Example $\rightarrow$ Octane/NIR-spectrum

# Theory

Jona

Motivation from multivariate regression (multivariate dgp).

# 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

# 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 $\Sigma_X$
- Let $\{\lambda_i \mid i = 1, \ldots, p\}$ be the corresponding **Eigenvalues** of $\Sigma_X$

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**:

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

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 $\xi_j$ 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).

$\Sigma_X$ 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 then called the functional principal components and the corresponding scores $\xi_i$ can be derived using the following equation.

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

## Simulation Setup & Application

Jona

- Compare b-spline / fourier regression chosen via criterion (cv/aic/...)
- Similar for fpca
- generate new curves from observed curves motivated by Karhunen-Loeve expansion
- Compare optimal variants with test and training sets
- Connect to Application

# Summary

Jona
Just summarize what we have done...

# further reading

Put footnotes here!