Scalar on Function Regression with Applications to Near-Infrared Spectography

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Presentation Day

Introduction

- **Near-Infrared** (NIR) **Spectroscopy** enables fast diagnostics by using the NIR region of the electromagnetic spectrum (from 780 nm to 2500 nm)
- Suited for field-monitoring / on-line analysis
- Spectroscopy results in high-dimensional dataset.
- This set of measurements serves as set of discretized approximations of smooth spectral curves
- Regression to determine relationship between octane rating and spectral curves

Theory

A simple functional dataset is given by

$$\{x_i(t_{j,i}) \in \mathbb{R} \mid i = 1, 2, ..., N,\ j = 1, 2, ..., J_i,\ t_{j,i} \in [T_1, T_2]\}$$

- Continuous underlying process, where $x_i(t)$ exists $\forall t \in [T_1, T_2]$
- Only observed at $x_i(t_{j,i})$
- Example: Gasoline dataset (60 x 400)
- Other Examples: Growth curves, financial data, human perception (pitch), ...

Random Function

A **Random Variable** is a function $X : \Omega \to \mathcal{S}$ which is defined on a common probability space $(\Omega, \mathcal{F}, \mathbb{P})$ where Ω is a probability space with a σ-algebra $\mathcal{F}$ and a probability measure $\mathbb{P}$.

- If $\mathcal{S} = \mathbb{R}$ then X is a random variable
- If $\mathcal{S} = \mathbb{R}^n$ then X is a random vector
- If $\mathcal{S}$ is a space of functions, X is called a **Random Function**

Random Function

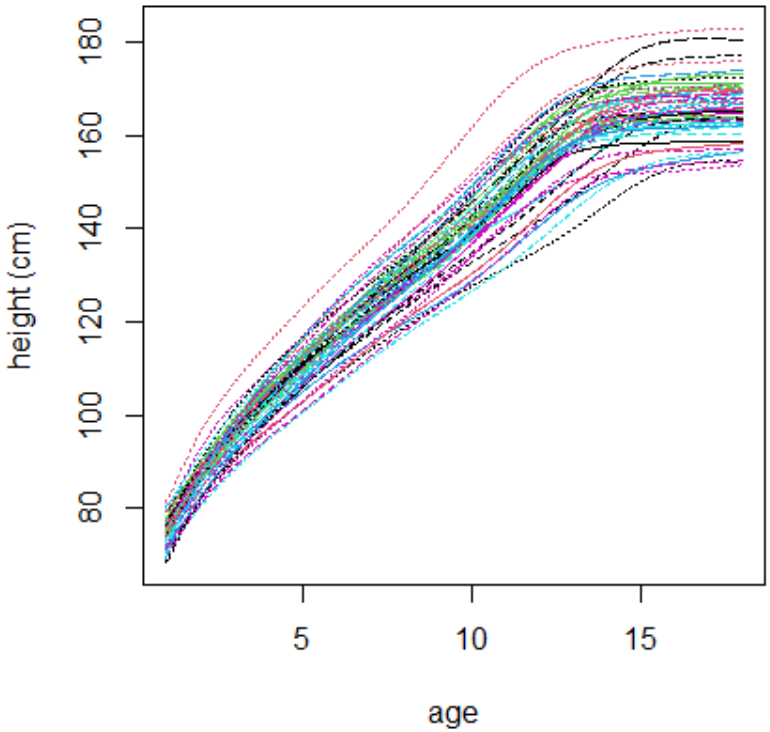
Let $\mathbb{E}$ be the index set and this can be described as

$$\{X(t,\omega) : t \in \mathbb{E}, \omega \in \Omega\},$$

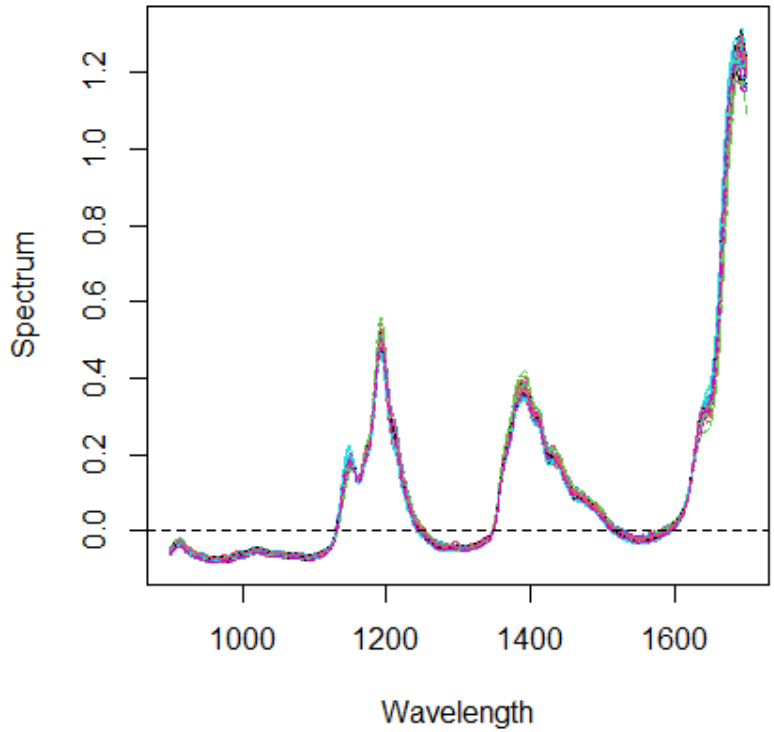
where $X(t,\cdot)$ is $\mathcal{F}$-measurable function on the sample space Ω.

- It can be shortened to $X(t)$ by omitting ω
- The function is realized when the $X(t)$ exists $\forall t \in \mathbb{E}$

Plots



Growth curves of
54 girls age 1-18



NIR spectrum of 60
gasoline samples

Square Integrable Function

If a function $f(t)$ satisfies

$$\int_0^1 (f(t))^2 \, dt < \infty$$

the function $f(t)$ is called **Square Integrable Function** written $f(t) \in \mathbb{L}^2[0,1]$.

- Without loss of generality, the interval is defined in $[0,1]$
- $\mathbb{L}^2$ is the set of all square integrable functions
- We focus on $\mathbb{L}^2[0,1]$ since the domain of our function is on the real line.

Square Integrable Function

Let $f, g \in \mathbb{L}^2[0,1]$, then

$$\langle f, g \rangle = \int_0^1 f(t)g(t)dt$$

Orthogonality of two different functions $\langle f, g \rangle = 0$

Basis Expansion

Basis Expansion is a linear combination of functions defining a function as described:

$$X_i(t) = \sum_{k=1}^{\infty} c_{ik}\phi_k(t) \approx \sum_{k=1}^{K} c_{ik}\phi_k(t), \quad i = 1, \ldots, n, \quad \forall t \in \mathbb{E}$$

where $\phi_k(t)$ is the k^{th} basis function of the expansion and c_{ik} is the corresponding coefficient. We truncate the basis at K to:

- make the function smoother
- replace the original curves $X_i(t)$ by a smaller collection of c_{nm}

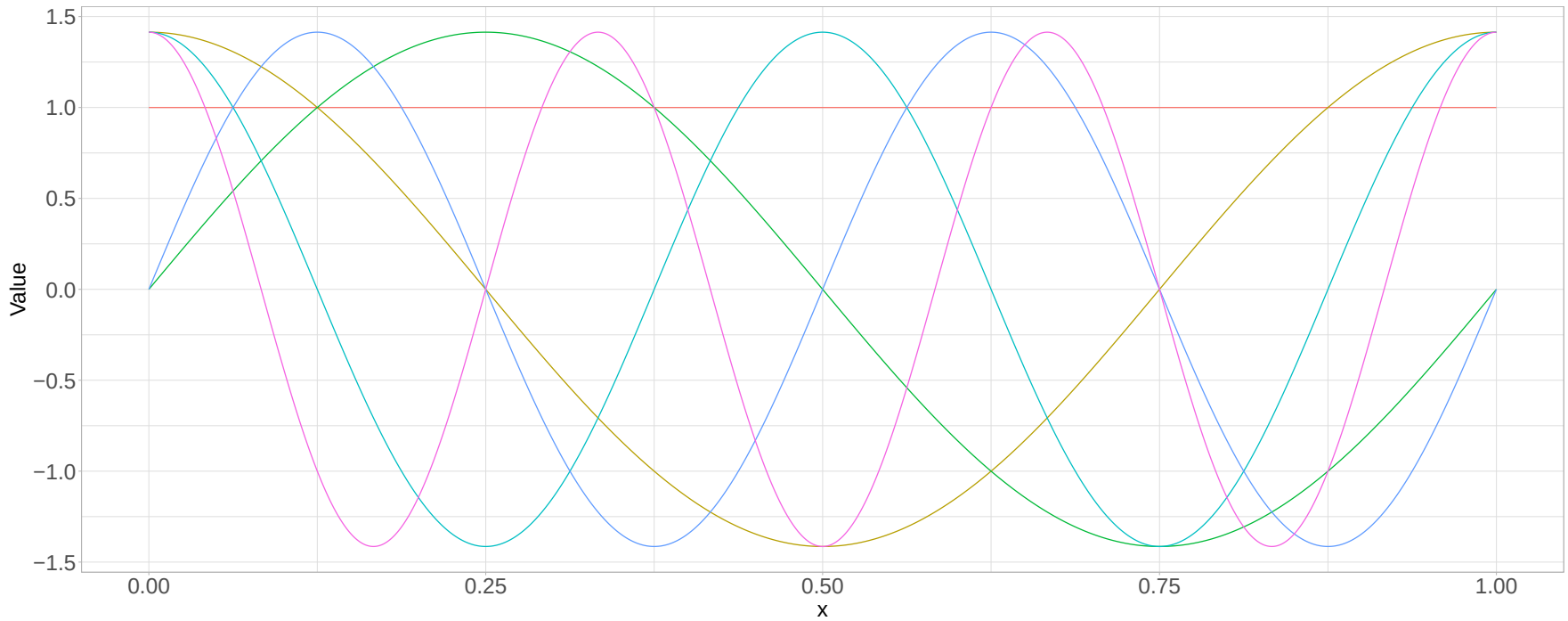
Two Typical Types of Basis Function

Fourier Basis Function is written as

$$f(x) = a_0 + \sum_{n=1}^{\infty} a_n cos(2\pi nx) + b_n sin(2\pi nx)$$

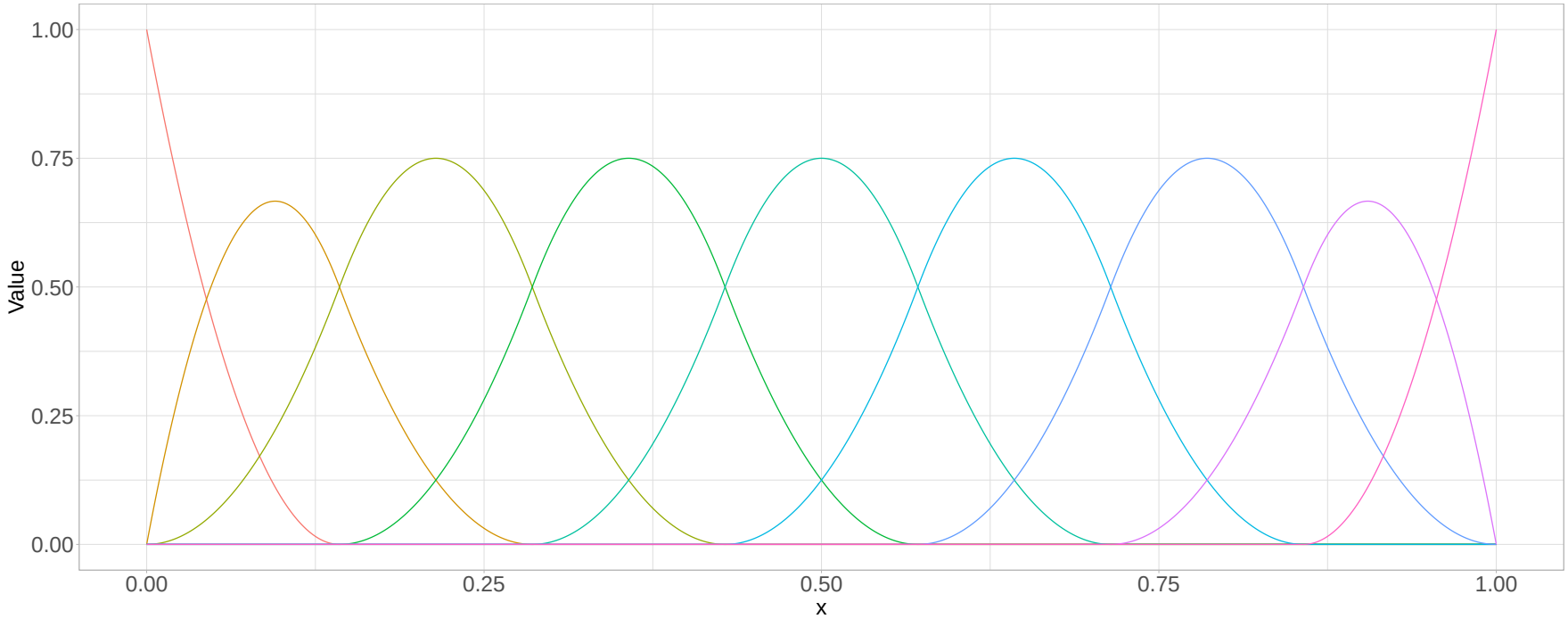
B-spline Basis Function is a flexible curve defined by degree and knots.
Each B-spline basis function, i-th B-spline basis function of degree p, $N_{i,p}(u)$ is defined on Cox-de Boor recursion formula.

Plots of Basis Functions



Fourier basis functions with order 9

Plots of Basis Functions



Bspline basis functions with order 9

Trade Off between Bias and Variance

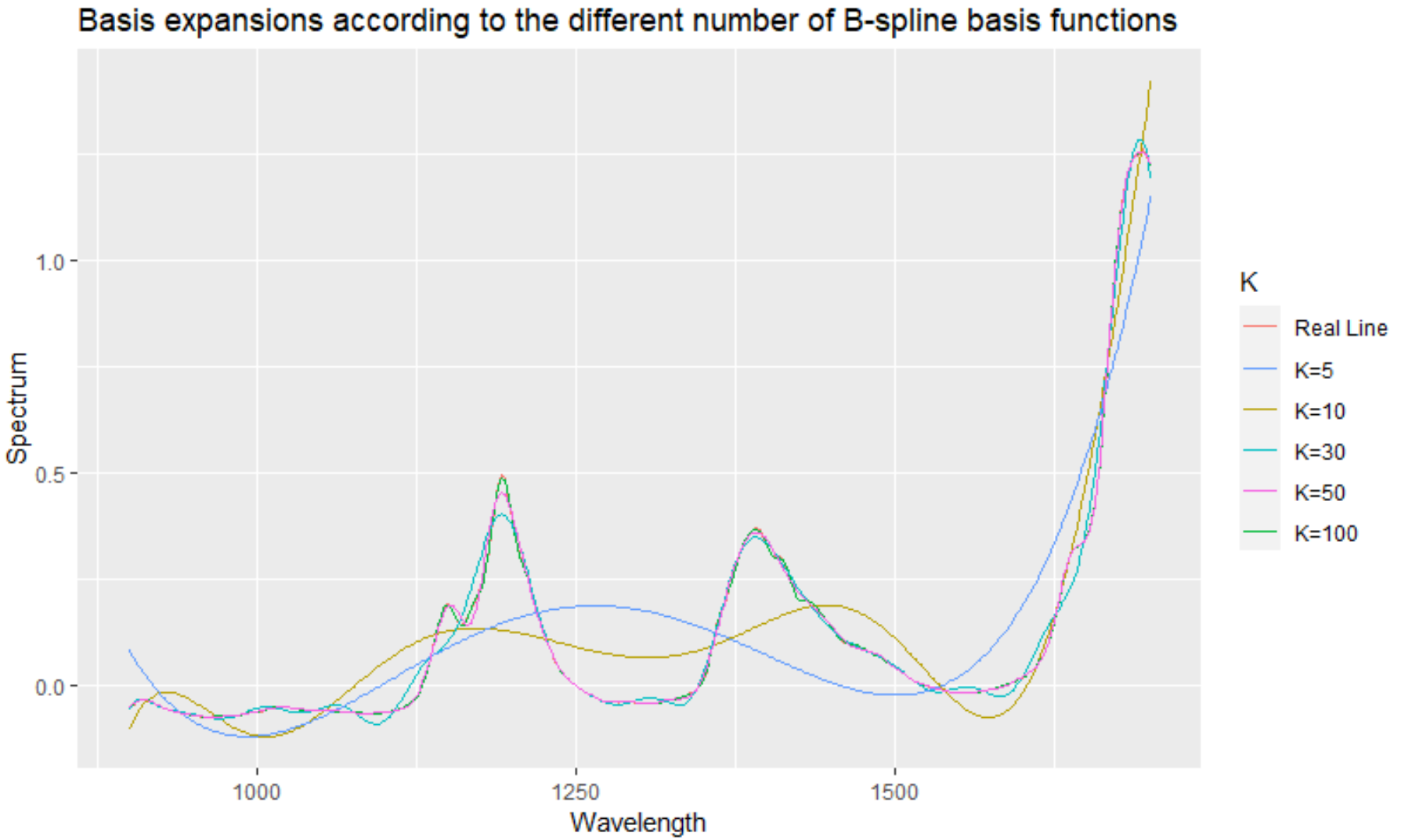
How do we choose the number K of basis functions?

$$\textbf{MSE}[\hat{x}(t)] = \textbf{Bias}^2[\hat{x}(t)] + \textbf{Var}[\hat{x}(t)]$$

Integrated Mean Squared Error

- The larger K, the better fit to the data with also fitting noise
- If K is too small, it would miss some significant information that we want to estimate

Trade Off between Bias and Variance



Estimation via Basis Representation

Assume the following **Data Generating Process**

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

- $Y(\omega)$ and $\epsilon(\omega)$ realize in $\mathbb{R}$ and $X(\omega)$ realizes in $\mathbb{L}^2[0,1]$

Let $\{\phi_i(t) \mid i = 1, \ldots, \infty\}$ be a basis of $\mathbb{L}^2[0,1]$ leading to the following representation of $\beta(t)$

$$\beta(t) = \sum_{j=1}^{\infty} c_j \phi_j(t) \approx \sum_{j=1}^{L} c_j b_j(t)$$

Estimation via Basis Representation

We can transform the data generating process into:

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

Where a $Z_j(\omega)$ is a **scalar random variable**.

Estimation via Basis Representation

Each combination of $x_i(t)$ and $\phi_j(t)$ gives us

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

- This allows us to write each observation in the data set as $(y_i, Z_{i,1}, Z_{i,2}, \dots)$
- Truncating the functional basis yields an approximation $(y_i, Z_{i,1}, Z_{i,2}, \dots, Z_{i,L})$

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

Estimation via Basis Representation

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

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

This is dependent on...

- The basis $(\phi_j(t))_{j\in\mathcal{I}}$ for the estimation of $\beta(t)$
- The truncation parameter L
- The basis $(\psi_j(t))_{j\in\mathcal{I}}$ used for the expansion of the observations
- The truncation parameter in the approximation of the observations K

Karhunen-Loéve Expansion

Mean Function:

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

Autocovariance Function:

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

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 $X(\omega)$ can be expressed in terms of its mean function and its Eigenfunctions:

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

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 is called the **Karhunen-Loéve Expansion** of $X(\omega)$ and the Eigenfunctions can serve as a basis.

Functional Principal Component Analysis

Principal Component Analysis 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:

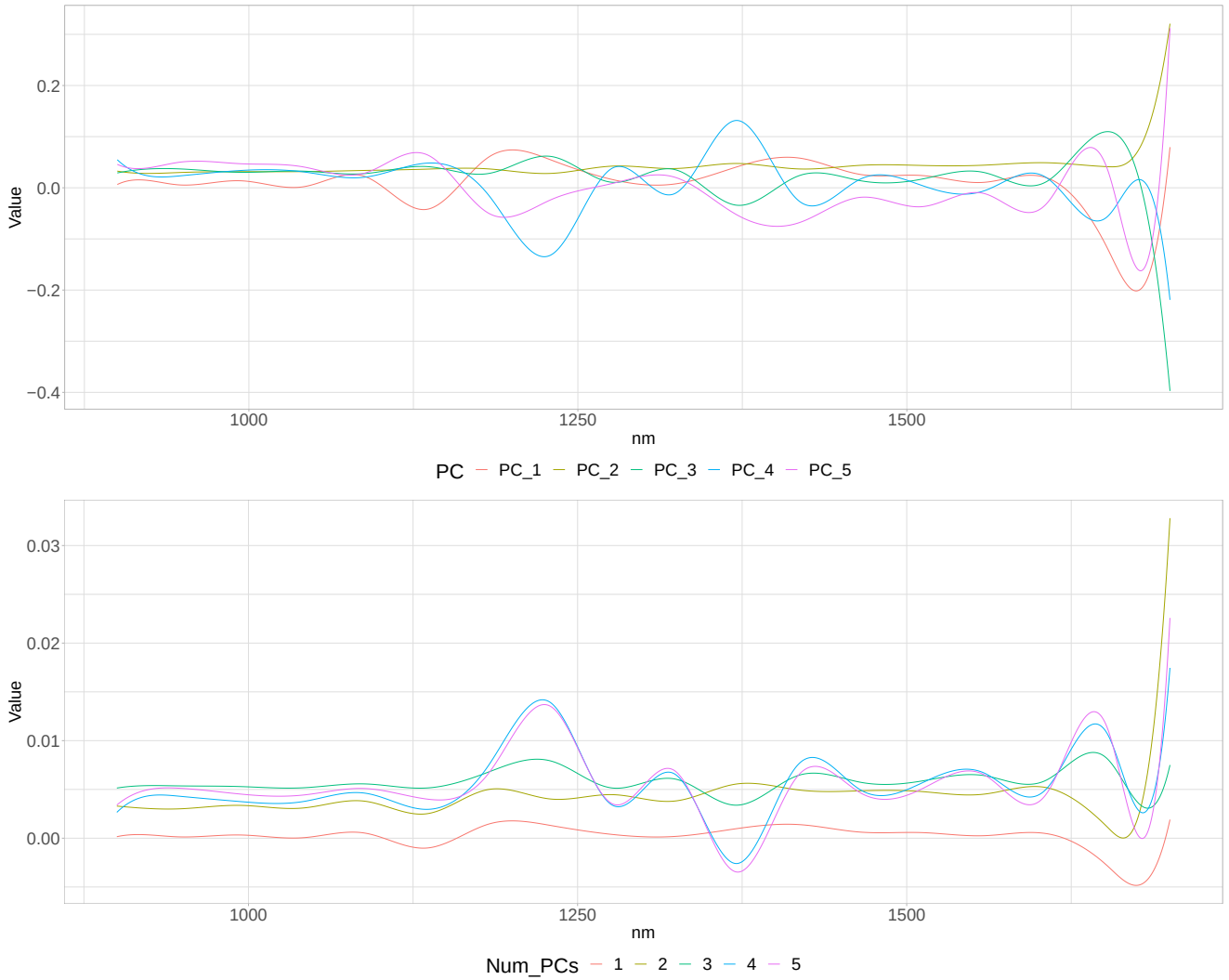
$$\int_0^1 \hat{c}(t,s)\hat{\nu}(s)\mathrm{d}s = \hat{\lambda}\hat{\nu}(t)$$

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



The math is for intuition. In practice there are problems and the fpc's are derived differently.

Simulation Setup

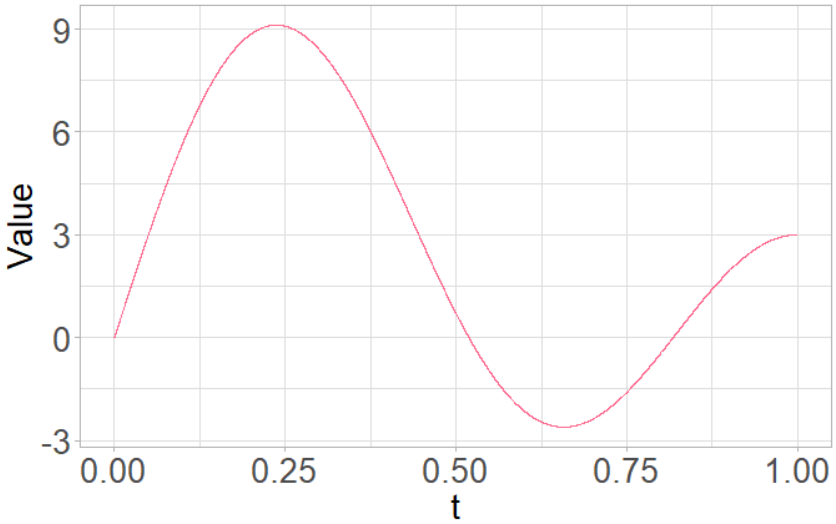
- Use the **Gasoline Dataset** (NIR-spectroscopy, 60×401) to predict octane ratings.
- Generate **similar curves** from gasoline dataset:

$$\tilde{X}(\omega)(t) = \hat{\mu}(t) + \sum_{j=1}^{J} \tilde{\xi}_j(\omega)\hat{\nu}_j(t)$$

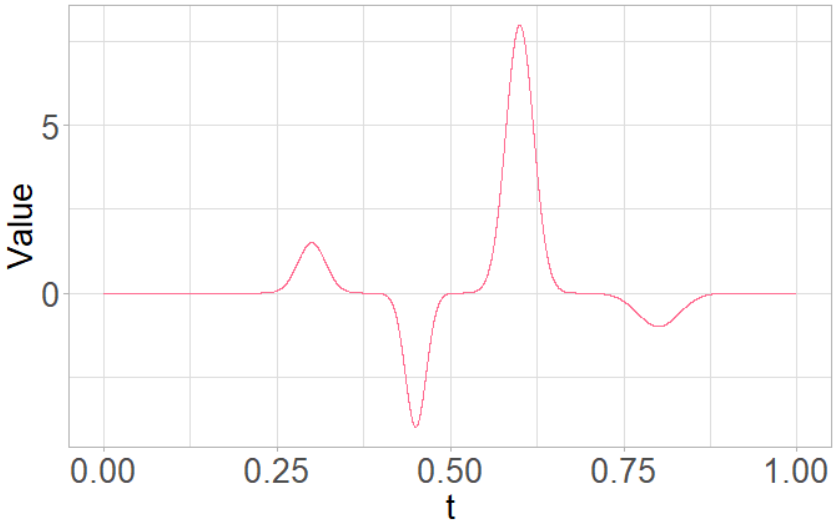
- $\tilde{\xi}_j \sim \mathcal{N}(0, \hat{\lambda}_j)$ and $\tilde{\xi}_j \perp\!\!\!\perp \tilde{\xi}_k$ for $j \neq k$
- Simplification: the ξ_j do not follow a normal
- $\tilde{X}(\omega)(t)$, $\hat{\mu}(t)$ and $\hat{\nu}_j(t)$ are approximated as vectors in $\mathbb{R}^{401}$.

Simulation Setup cont.

Following **Reiss and Ogden (2007)**, let $f_1(t)$ and $f_2(t)$ be two coefficient functions:



$f_1(t)$, smooth function



$f_2(t)$, bumpy function

Simulation Setup cont.

Let

$$Y_{1,f} = \langle NIR, f \rangle + Z \left(\frac{var(\langle NIR, f \rangle)}{0.9} - var(\langle NIR, f \rangle) \right)$$

$$Y_{2,f} = \langle NIR, f \rangle + Z \left(\frac{var(\langle NIR, f \rangle)}{0.6} - var(\langle NIR, f \rangle) \right)$$

where $Z \sim \mathcal{N}(0, 1)$ be two responses for $f \in \{f_1(t), f_2(t)\}$.

- Four combinations with different number of cubic basis-function $n_{basis} \in (4, 5, ..., 25)$ and fourier functions $(1, 3, ..., 25)$ to perform regression using basis expansion and the FPCR approach.
- Compare results via criteria (CV, Mallows CP,...)

Simulation Results

- add results here!

Application setup

- Use insights from the simulation study to uncover dependence.
- Similar setup, but using only bspline basis expansion and initial 60 spectral curves.
- Validation set approach: Scores of test data needs to be estimated by the training data.
- Report results by MSE scaled by variance.

Summary

- Concepts of functional data:
  - See dataset as smooth curve than as set of discrete measurements.
  - Theory of Random Functions, motivated from random variable.
  - Basis expansion and its Bias-Variance tradeoff.
  - Scalar on Function Regression via Basis Expansion.
  - Functional principal component Analysis and FPCR.
- Simulation study results: specification depends on function and signal-to-noise ratio
- Guided through application to predict octane ratings.

Thank you for your time!

Further Reading

Put footnotes here!

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 $i \neq j$

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 $i \neq j$