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 $x_i(t_{j,i})$
- Growth curves, financial data, human perception (pitch), ...
- To abstract information from the curves, they must be interpretable!

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

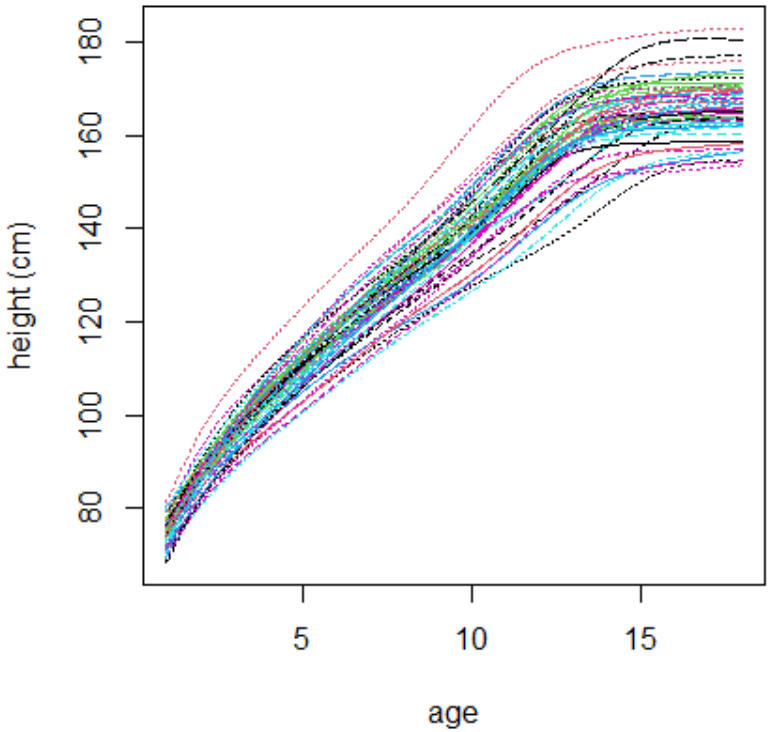
Let $\mathbb{E}$ be the index set and this can be described as

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

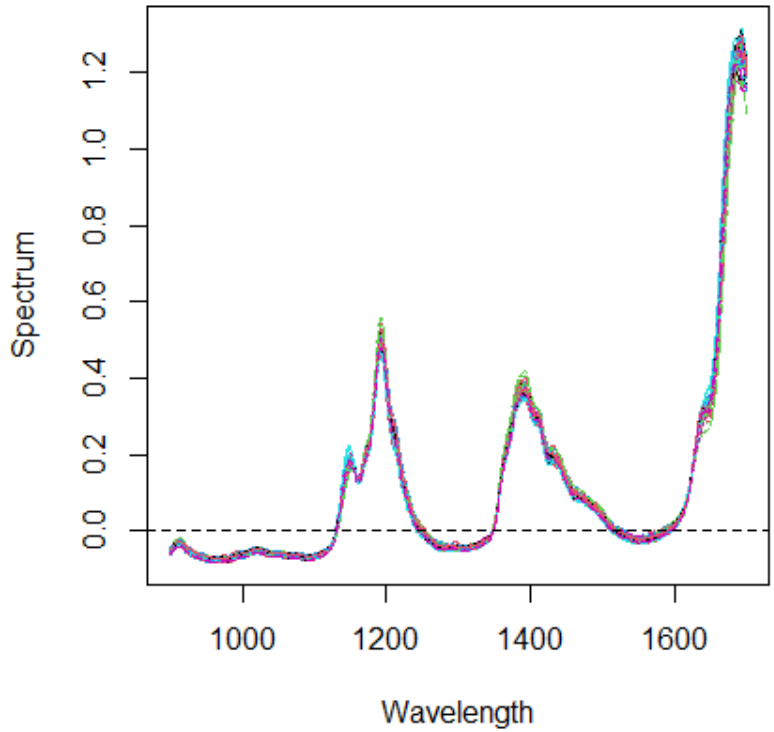
where $X(t,\cdot)$ is $\mathcal{F}$-measurable function on the sample space Ω.

- 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}

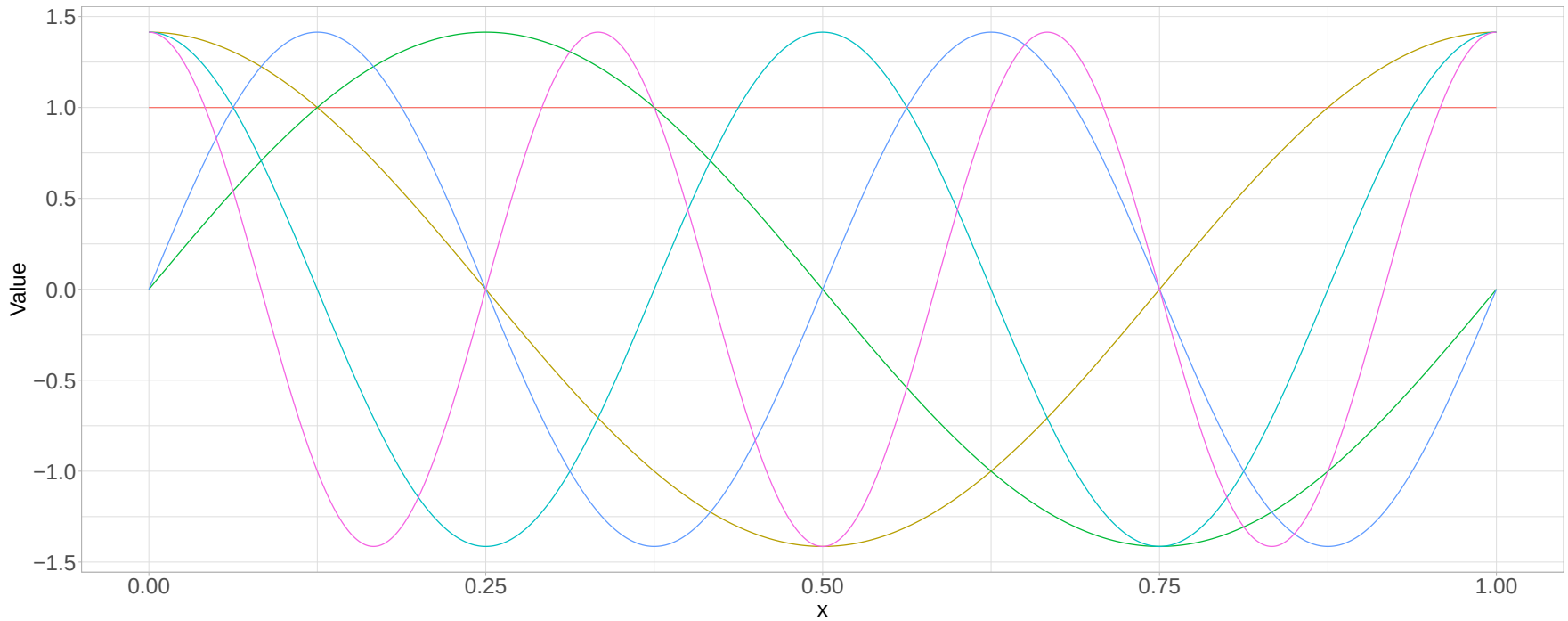
Two Typical Types of Basis Function

Fourier Basis Function is written as

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

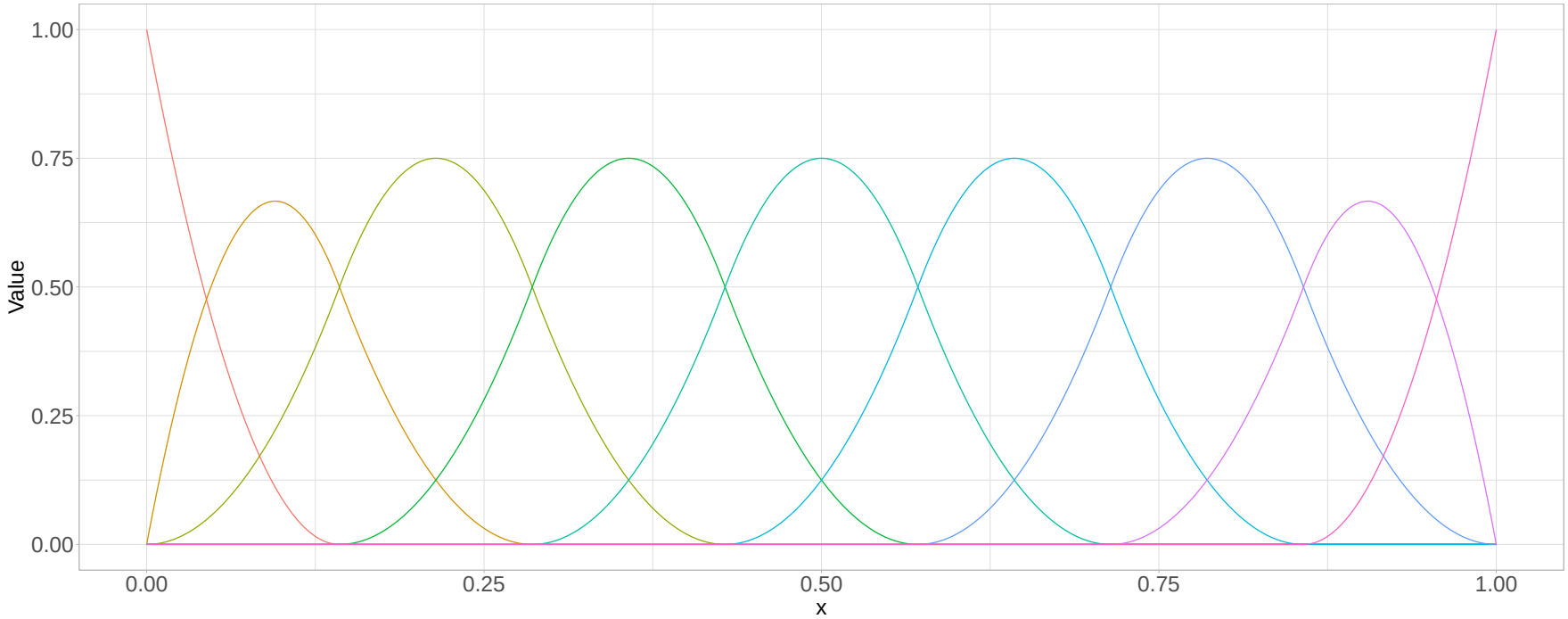
B-spline Basis Function is a flexible curve defined by degree and knots.
Each B-spline basis function, i-th B-spline basis function of degree p, $N_{i,p}(u)$ is defined on Cox-de Boor recursion formula.

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

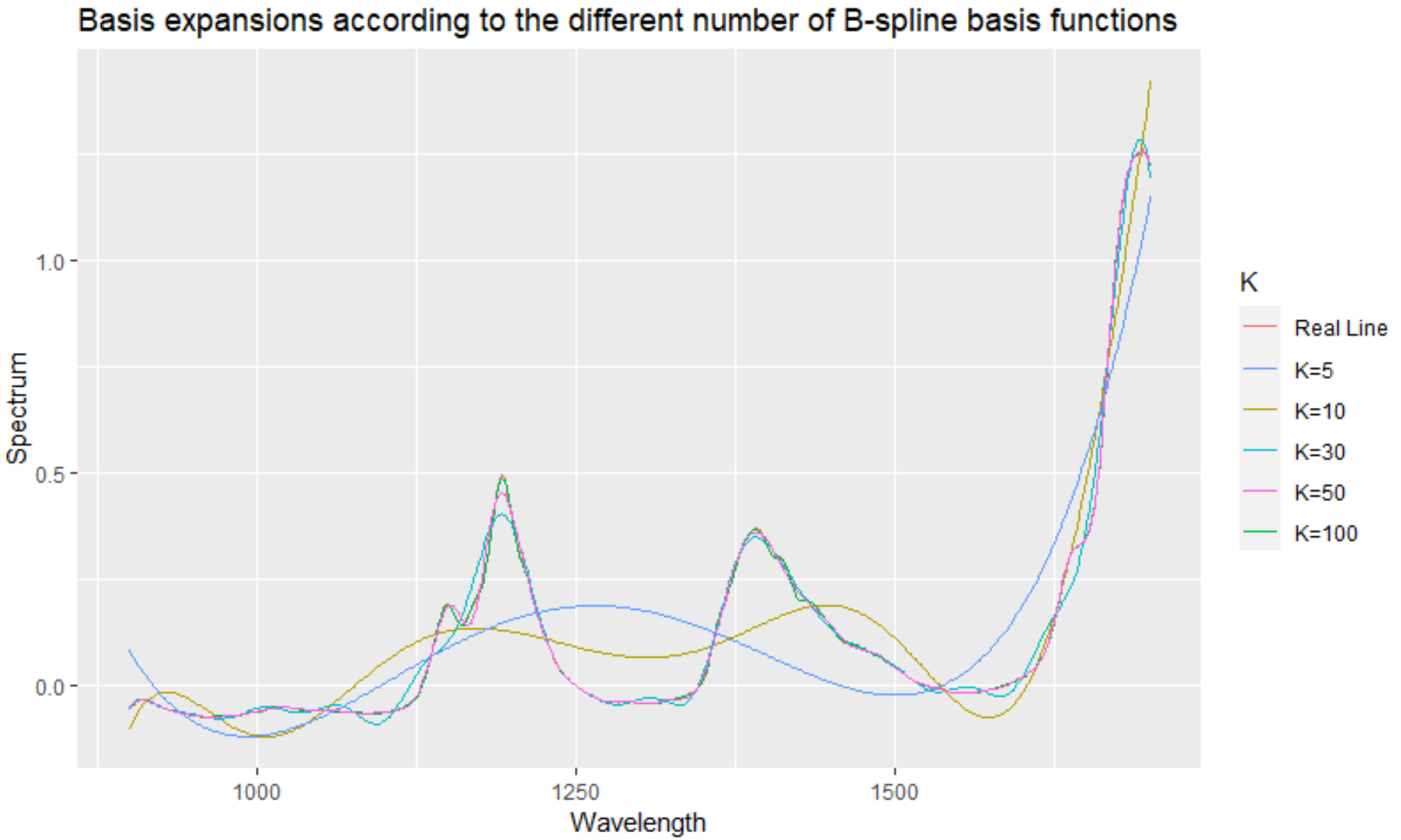
How do we choose the number K of basis functions?

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

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:

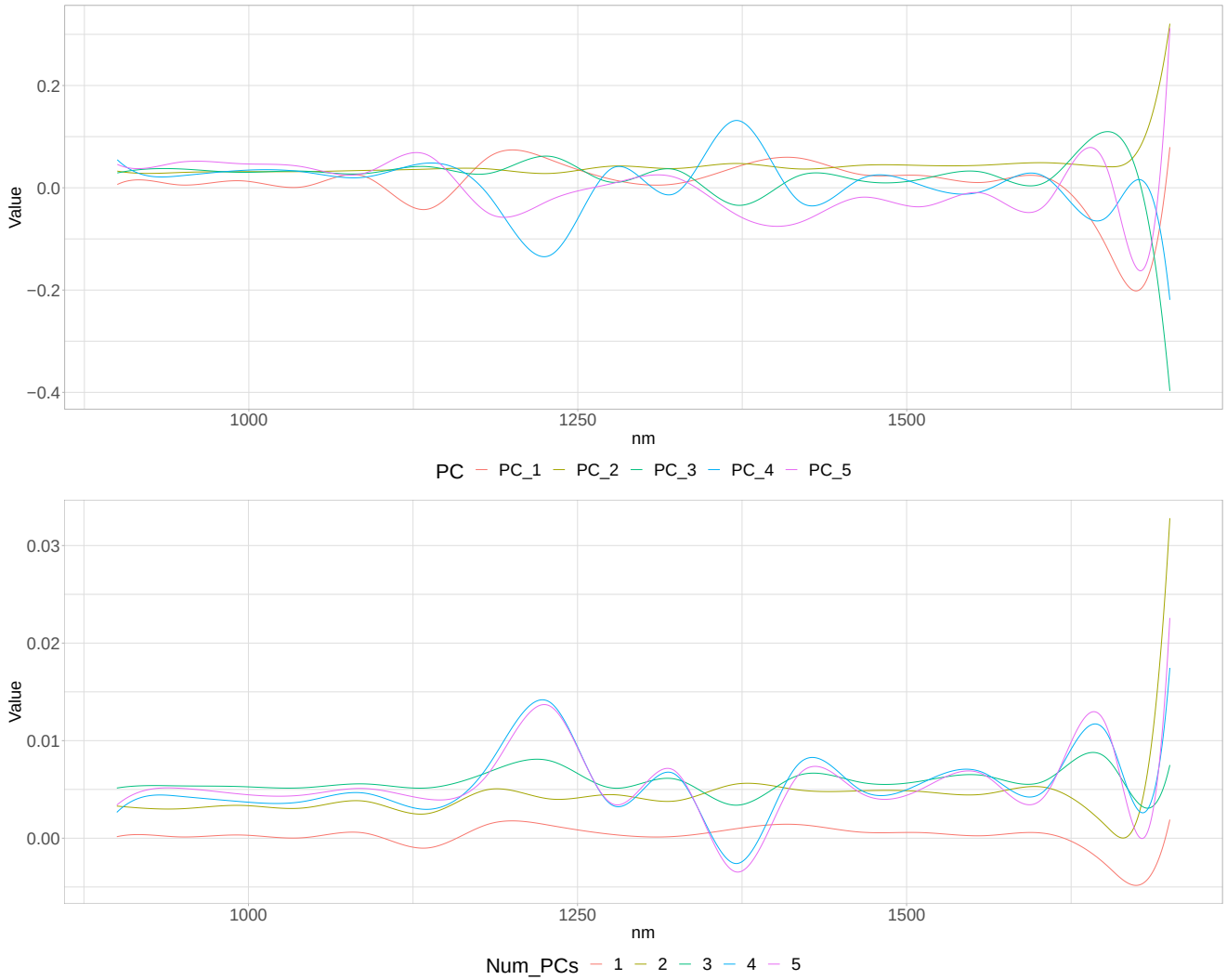
$$\int_0^1 \hat{c}(t,s)\hat{\nu}(s)\mathrm{d}s = \hat{\lambda}\hat{\nu}(t)$$

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 & Application

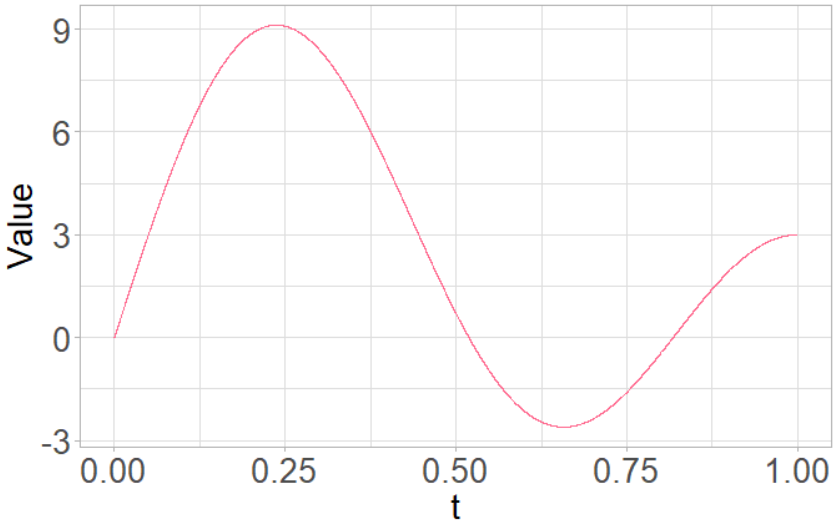
- Use the **Gasoline Dataset** (NIR-spectroscopy, 60×401) to predict octane ratings.
- Generate **similar curves** from gasoline dataset:

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

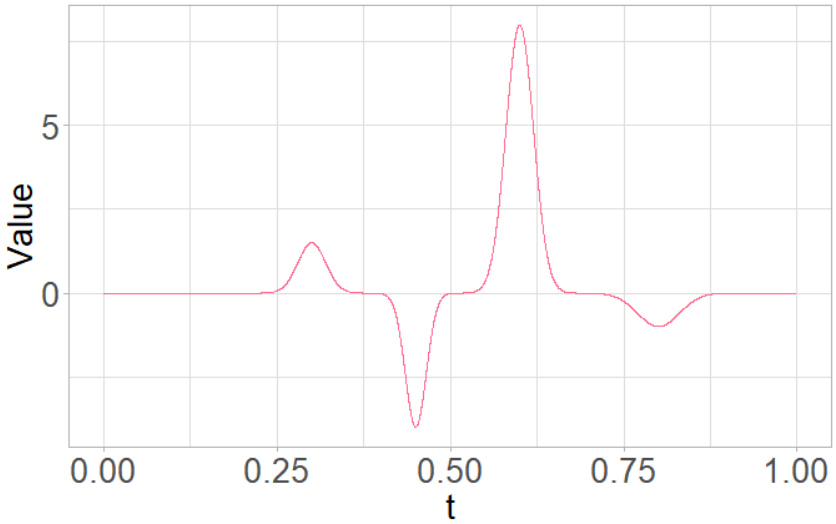
- $\tilde{\xi}_j \sim \mathcal{N}(0, \hat{\lambda}_j)$ and $\tilde{\xi}_j \perp\!\!\!\perp \tilde{\xi}_k$ for $j \neq k$
- Simplification: the ξ_j do not follow a normal
- $\tilde{X}(\omega)(t)$, $\hat{\mu}(t)$ and $\hat{\nu}_j(t)$ are approximated as vectors in $\mathbb{R}^{401}$.

Simulation Setup & Application 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 & Application cont.

Let

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

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

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 $n_{basis} \in (5, 6, ..., 25)$ 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...

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 $i \neq j$