Scalar on Function Regression with Applications to Near-Infrared Spectroscopy

Jonathan Willnow, Jakob Juergens, Jonghun Baek

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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

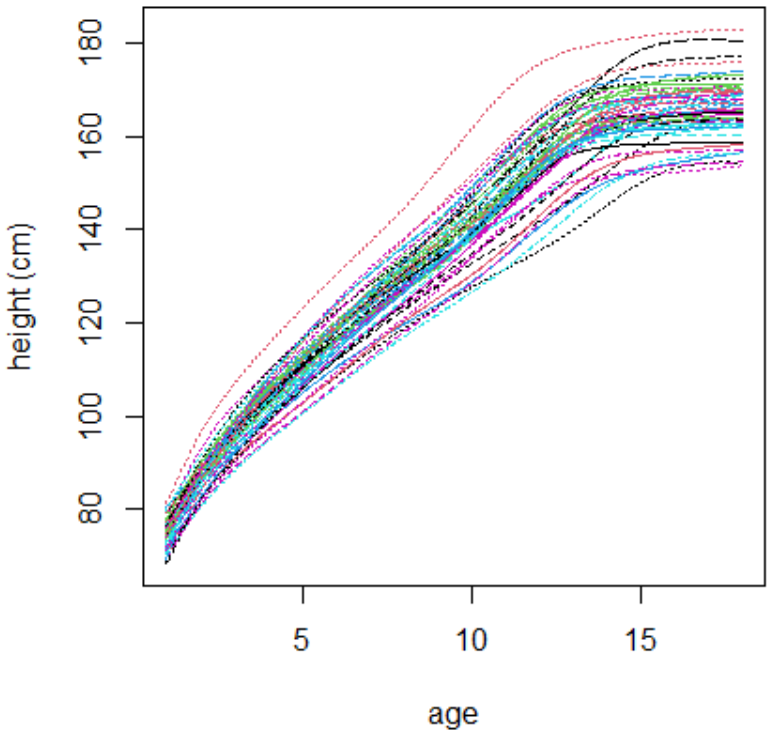
Let $\mathbb{E}$ be the index set and this can be described as

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

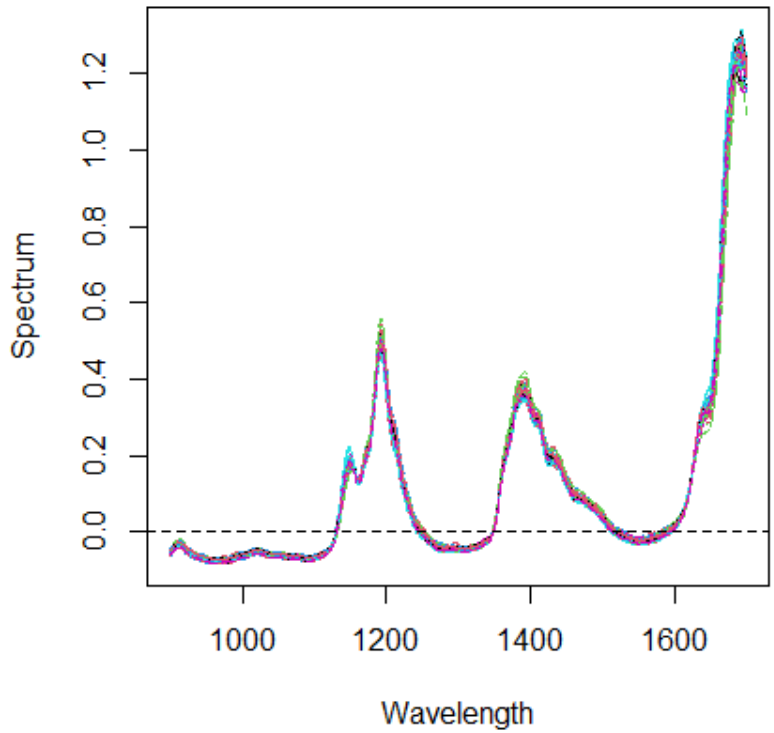
where $X(t, \cdot)$ is $\mathcal{F}$-measurable function on the sample space Ω.

- 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.

Square Integrable Function

Let $f, g \in \mathbb{L}^2[0,1]$, then we can define inner product by

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

- Orthogonality of two different functions with $\langle f, g \rangle = 0$
- Distance between functions

Basis Expansion

Basis Expansion is a linear combination of functions 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}

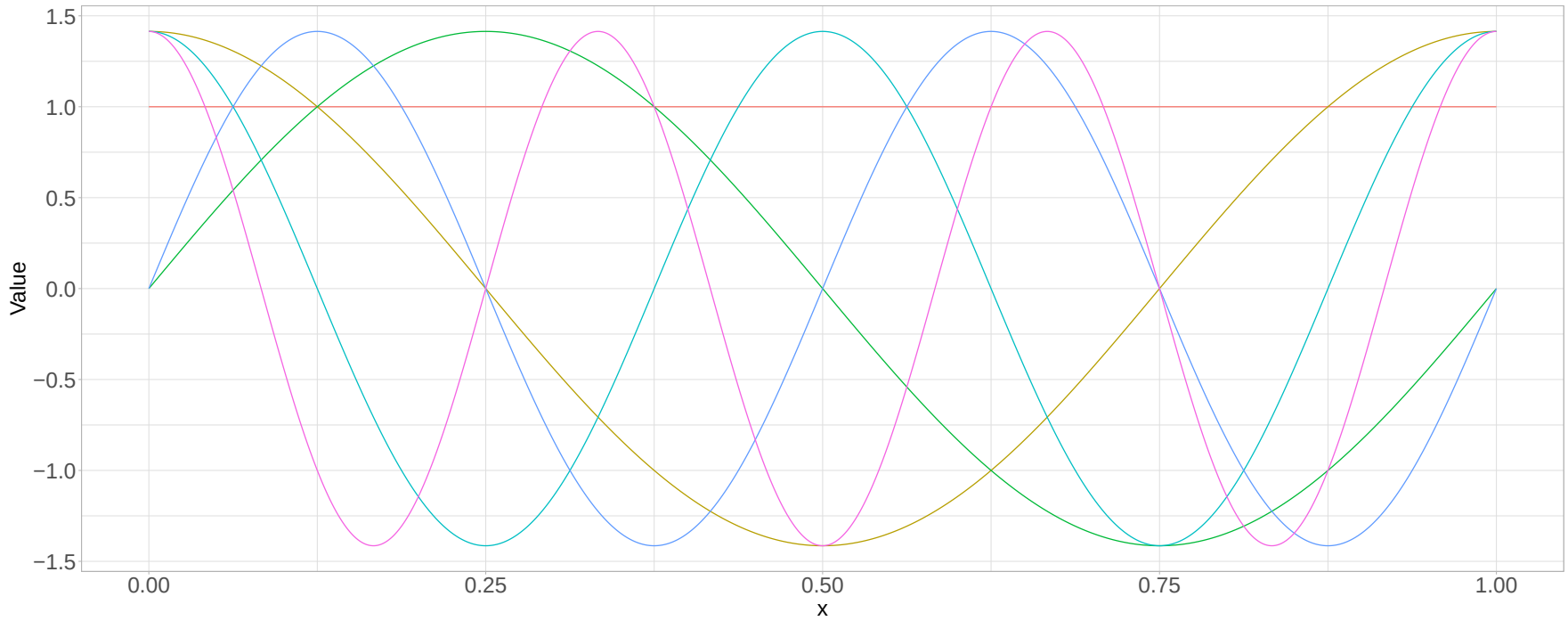
Two Typical Types of Basis Function

Fourier Basis Function is an element of the set:

$$\{\sqrt{2}sin(2\pi nx|n \in \mathbb{N})\} \cup \{\sqrt{2}cos(2\pi nx|n \in \mathbb{N})\} \cup \{1\}$$

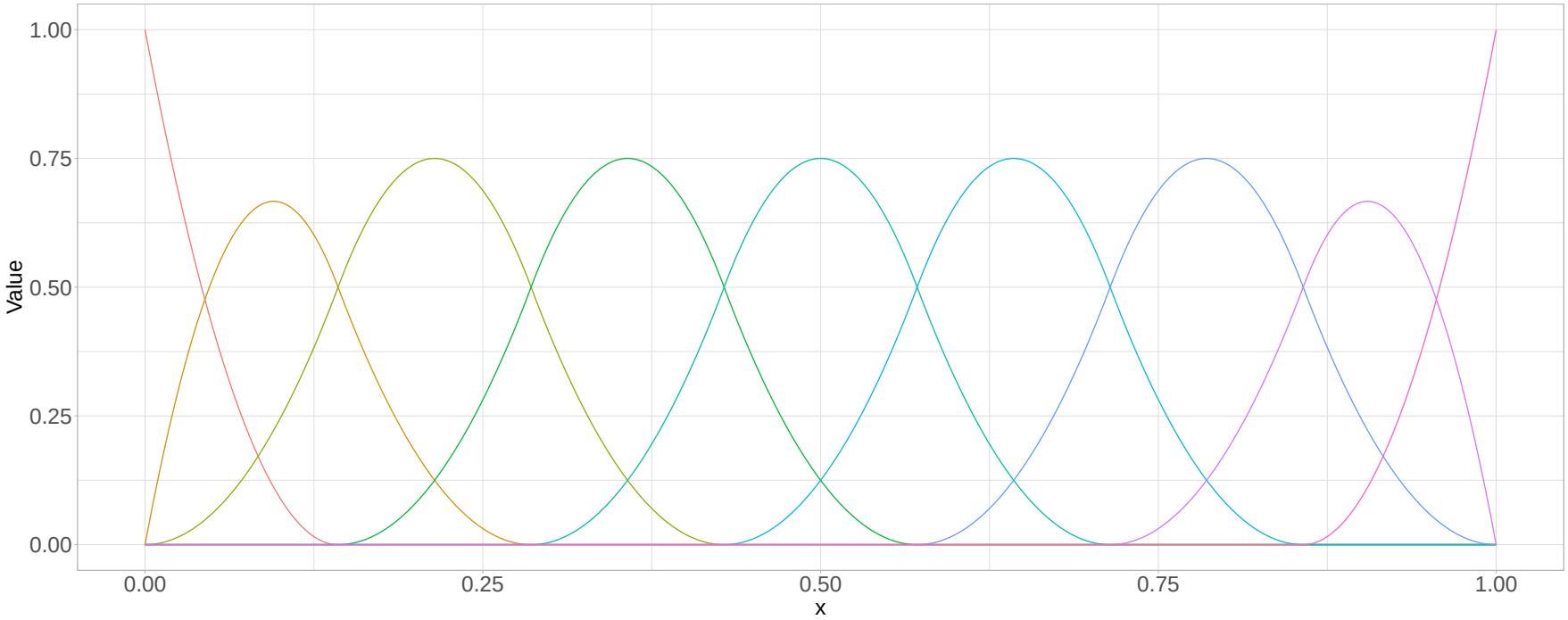
B-spline Basis Function is a polynomial function defined by order and knots.

Plots of Basis Functions



Fourier basis functions

Plots of Basis Functions



Bspline basis functions

Trade Off between Bias and Variance

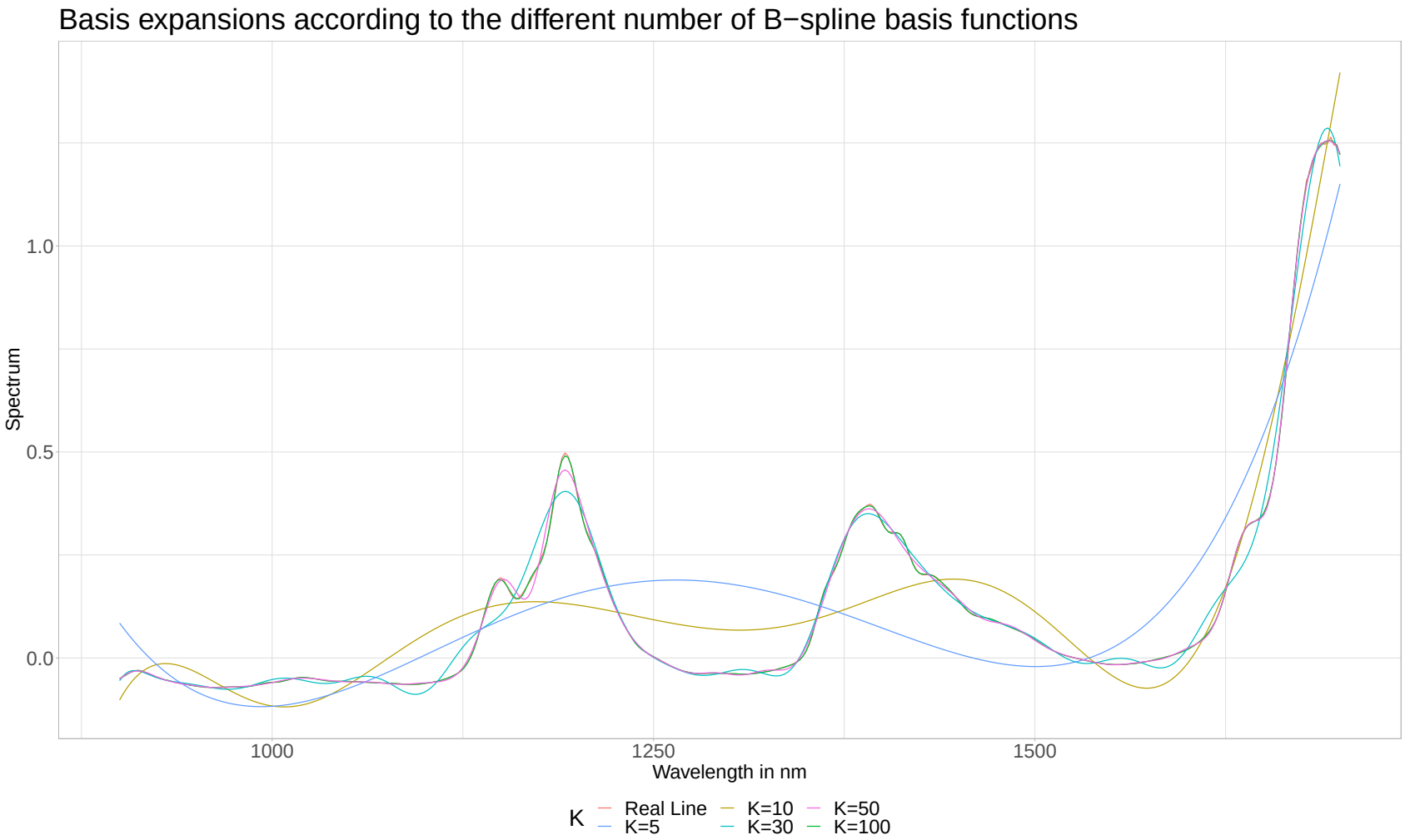
How do we choose the number K of basis functions?

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

$$\textbf{MISE}[\hat{X}] = \int_0^1 \textbf{MSE}[\hat{X}(t)]dt$$

- The larger K, the better fit to the data, but also more fitting noise
- If K is too small, the expansion would miss some significant information

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 $\beta(t)$

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

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

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

- 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.

▸ Spectral Representation of Random Vectors

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:

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

Empirical Autocovariance Function:

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

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:

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

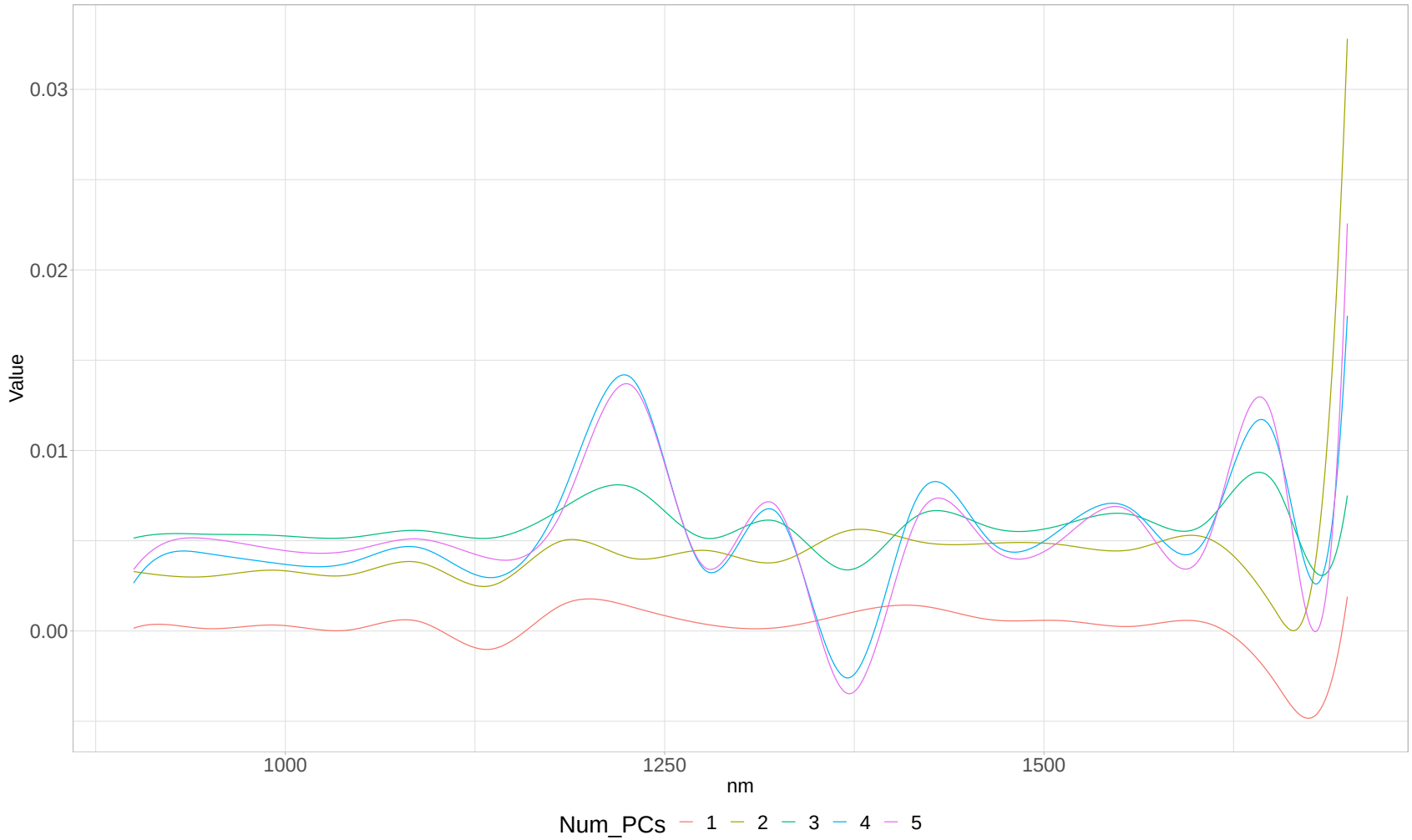
The $\{\hat{\nu}_i(s) \mid i \in \mathcal{I}\}$ are called **Functional Principal Components** and can serve as a basis for representing the original curves.

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

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

▸ PCA for Random Vectors

FPCA - Plot



Simulation Setup

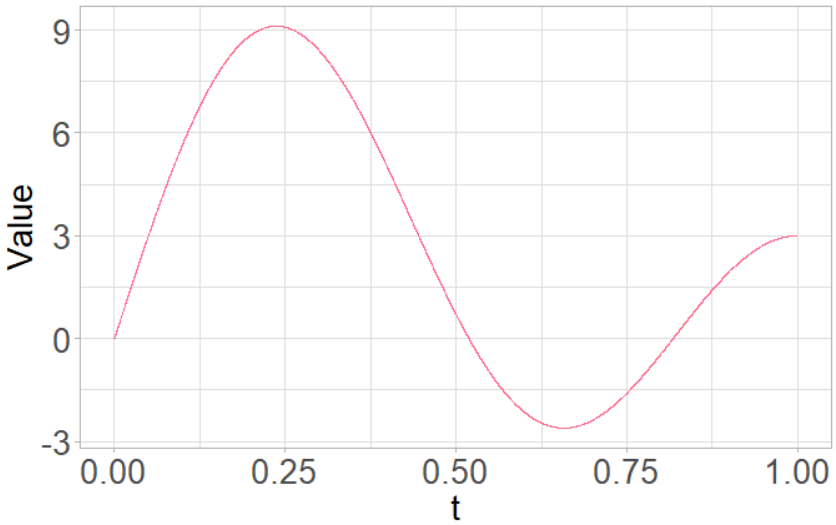
- Use the **Gasoline Dataset** (NIR-spectroscopy, 60×401) to predict octane ratings.
- Generate **similar curves** from gasoline dataset:

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

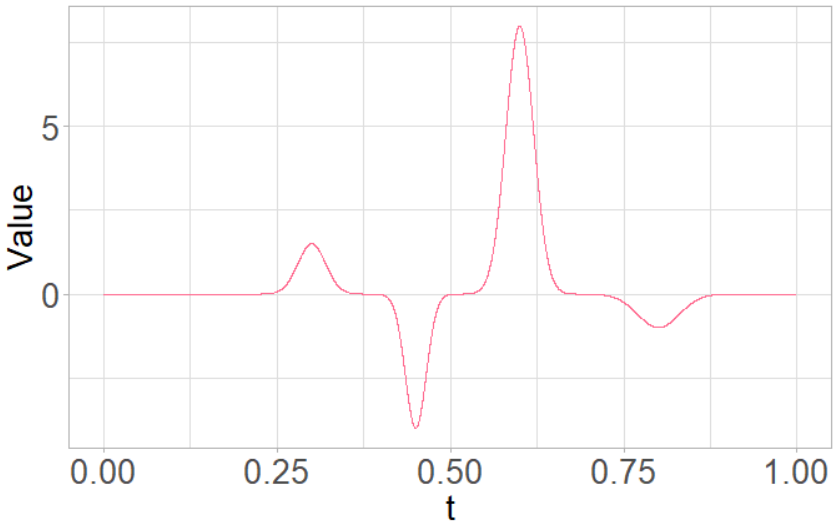
- $\tilde{\xi}_j \sim \mathcal{N}(0, \hat{\lambda}_j)$ and $\tilde{\xi}_j \perp\!\!\!\perp \tilde{\xi}_k$ for $j \neq k$
- Simplification: the ξ_j do not follow a normal
- $\tilde{X}(\omega)(t)$, $\hat{\mu}(t)$ and $\hat{\nu}_j(t)$ are approximated as vectors in $\mathbb{R}^{401}$.

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

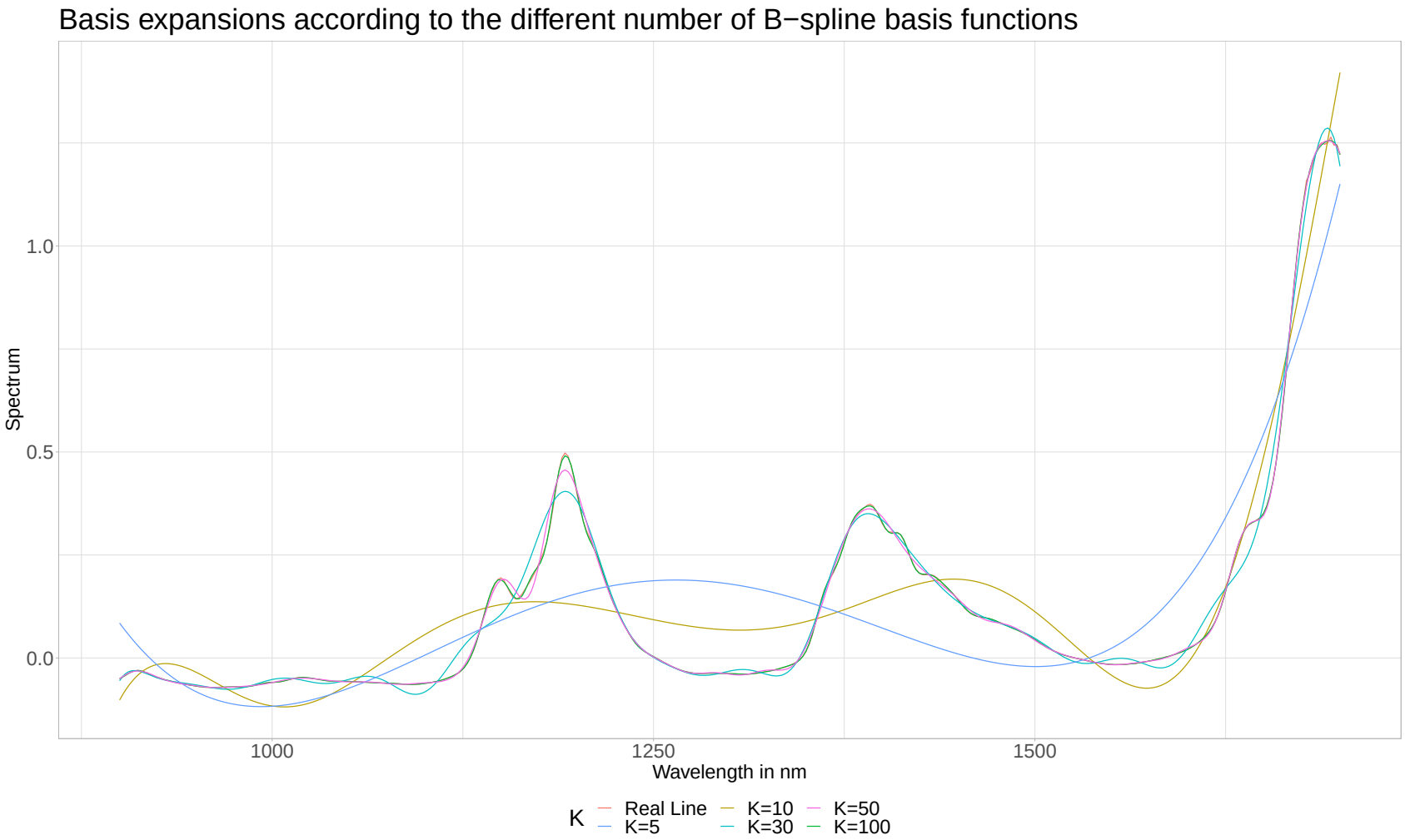
$$Y_{1,f} = \langle NIR, f \rangle + Z \left(\frac{var(\langle NIR, f \rangle)}{0.9} - var(\langle NIR, f \rangle) \right)$$

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

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,...)

Recap: Trade Off between Bias and Variance



Simulation - Interpretation of results

- Basis expansion regression
  - Smooth true coefficient functions requires smaller number of n_{basis} and vis versa.
  - Setup with higher noise requires smoother function.
  - Bsplines perform overall better.
- FPCR
  - Two PC enough to explain variation.
  -

Simulation Results - bspline basis expansion

f1_e1_spline	f1_e2_spline	f2_e1_spline	f2_e2_spline	n_basis
2.1318	71.71	0.6082	1.5345	4
2.0076	71.9395	0.3427	1.2906	5
1.9937	72.2563	0.2456	1.2014	6
2.0365	73.7857	0.2797	1.2495	7
2.1861	79.0485	0.1044	1.1458	8
2.0511	74.1784	0.0356	1.0217	9
2.1052	76.1884	0.0297	1.0393	10
2.1012	76.4031	0.0296	1.0425	11
2.3815	86.1707	0.037	1.1819	12
2.2114	80.6208	0.0363	1.1024	13
2.4495	87.6977	0.038	1.2126	14
2.2887	83.4755	0.0315	1.1363	15
2.5491	93.593	0.0352	1.2652	16
2.5514	93.3074	0.0352	1.2661	17
2.7516	100.5562	0.038	1.362	18
3.0243	109.9876	0.041	1.4813	19
3.4255	122.396	0.0472	1.6854	20

Simulation Results - fourier basis expansion

f1_e1_spline	f1_e2_spline	f2_e1_spline	f2_e2_spline	n_basis
0	0	0	0	1
2.0292	72.0085	0.512	1.4747	3
2.022	72.6017	0.1616	1.1375	5
2.0355	73.1836	0.0293	0.9907	7
2.062	73.9631	0.029	0.9994	9
2.0881	75.0921	0.0291	1.0139	11
2.0997	75.9422	0.0294	1.0291	13
2.1087	76.7123	0.0298	1.0371	15
2.1301	77.4908	0.03	1.0398	17
2.1535	78.3943	0.0303	1.0509	19
2.1775	79.2058	0.0307	1.0617	21
2.2058	80.3801	0.031	1.077	23
2.2372	81.509	0.0315	1.0905	25

Simulation Results - bspline FPCR ($n_{harm} = 2$)

f_1, error 1	f_1, error 2	f_2, error 1	f_2, error 2	expl. variance	n_basis
2.9163	10.8768	0.9599	1.6431	1	4
2.345	10.585	0.8649	1.5631	0.9776	5
2.4187	10.6889	0.8739	1.5759	0.9556	6
2.4971	10.7287	0.8625	1.5723	0.9472	7
2.5799	10.6971	0.8716	1.575	0.9239	8
2.6828	10.7669	0.853	1.5661	0.9178	9
2.825	10.7906	0.8304	1.5622	0.8976	10
2.9082	10.7774	0.8237	1.5424	0.906	11
2.9519	10.8126	0.8286	1.5561	0.9036	12
2.9972	10.8221	0.8404	1.5551	0.9052	13
2.9755	10.7706	0.8396	1.5614	0.9074	14
2.9762	10.7946	0.8476	1.557	0.9058	15
2.9627	10.8067	0.8609	1.5615	0.9061	16
2.9621	10.7707	0.857	1.5628	0.906	17
2.9929	10.8315	0.8536	1.5632	0.8935	18
2.9576	10.7894	0.8676	1.5656	0.901	19
2.9835	10.8445	0.8514	1.5612	0.8934	20

Simulation Results - fourier FPCR ($n_{harm} = 2$)

f_1, error 1	f_1, error 2	f_2, error 1	f_2, error 2	expl. variance	n_basis
0	0	0	0	0	1
2.2059	11.2438	0.8768	1.5528	0.9846	3
2.2148	11.2567	0.8227	1.5215	0.9584	5
2.2635	11.2662	0.8828	1.5563	0.9489	7
2.2721	11.2692	0.8811	1.5531	0.9439	9
2.2797	11.2574	0.879	1.555	0.9397	11
2.3039	11.2708	0.8887	1.5591	0.9421	13
2.3248	11.2898	0.8743	1.5514	0.9283	15
2.3798	11.2957	0.875	1.5511	0.9182	17
2.4233	11.3049	0.8632	1.5453	0.9167	19
2.4589	11.3094	0.8619	1.5432	0.9133	21
2.5306	11.331	0.8562	1.5408	0.9082	23
2.5752	11.3272	0.8531	1.5393	0.9062	25

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

Further Reading:

Gy. Bohács, Z. Ovádi, A. Salgó (1998). "Prediction of Gasoline Properties with near Infrared Spectroscopy". In: *Journal of near infrared spectroscopy.* 6, pp. 341–348.

Li, Yuanpeng et al. (2020). "Early Diagnosis of Type 2 Diabetes Based on Near-Infrared Spectroscopy Combined With Machine Learning and Aquaphotomics". In: *Frontiers in Chemistry* 8, p. 1133. ISSN: 2296-2646. DOI: 10.3389/fchem.2020.580489. URL: https://www.frontiersin.org/article/10.3389/fchem.2020.580489.

Reiss, Philip T. and R. Todd Ogden (2007). "Functional Principal Component Regression and Functional Partial Least Squares". In: *Journal of the American Statistical Association* 102.479, pp. 984–996. ISSN: 0162-1459. DOI: 10.1198/016214507000000527.

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

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