Scalar on Function Regression with Applications to Near-Infrared Spectroscopy

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Introduction

Near-Infrared (NIR) **Spectroscopy** enables fast diagnostics by using the NIR region of the electromagnetic spectrum

- Spectroscopy results in high-dimensional dataset: Gasoline dataset (60 x 401)
- This set of measurements serves as set of discretized approximations of smooth spectral curves

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

- Continuous underlying process where $x_i(t)$ exists $\forall t \in [T_1, T_2]$ but is only observed at $t_{j,i}$
- Regression to determine relationship between octane rating and spectral curves

Random Function

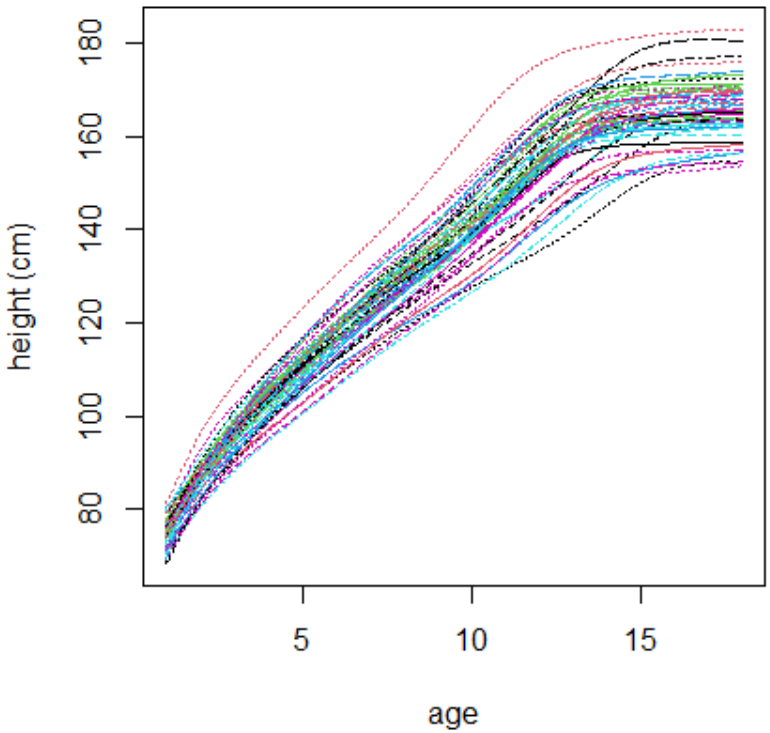
A **Random Variable** is a function $X : \Omega \to \mathcal{S}$ which is defined on a common probability space $(\Omega, \mathcal{F}, \mathbb{P})$ where Ω is a probability space with a σ-algebra $\mathcal{F}$ and a probability measure $\mathbb{P}$.

- 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**

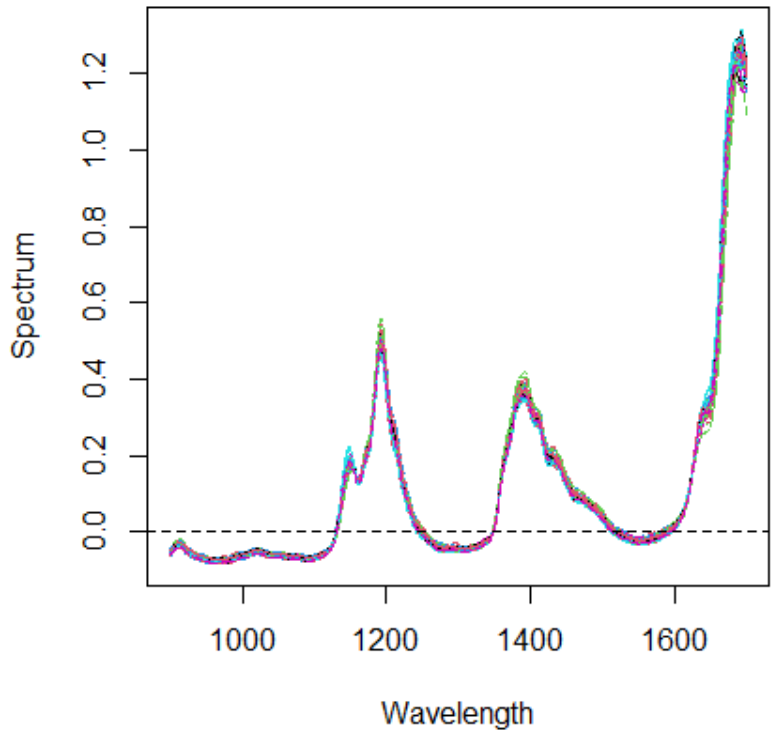
A **Realization** of a random function $X(\omega)$ is a function

$$x_0(t) = X(\omega_0)(t) \quad t \in \mathbb{E},\ \omega_0 \in \Omega$$

Plots



Growth curves of
54 girls age 1-18



NIR spectrum of 60
gasoline samples

Square Integrable Function

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

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

- Without loss of generality, the interval is defined in $[0,1]$.

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 $\langle f, g \rangle = 0$

Square Integrable Function

A natural **Norm** to be defined on $\mathbb{L}^2[0,1]$ is the following norm induced by the inner product.

$$||f|| = \sqrt{\langle f, f \rangle} = \sqrt{\int_0^1 f(t)^2 dt}$$

This norm naturally induces a **Distance** on $\mathbb{L}^2[0,1]$.

$$d(f,g) = ||f-g|| = \sqrt{\langle f-g, f-g \rangle} = \sqrt{\int_0^1 [f(t)-g(t)]^2 \, dt}$$

Basis Expansion

Basis Expansion is a linear combination of functions as described:

$$x_i(t) = \sum_{j \in \mathcal{I}} c_{i,j}\phi_j(t) \approx \sum_{j=1}^{L} c_{i,j}\phi_j(t), \quad i = 1, \ldots, n, \quad \forall t \in \mathbb{E}$$

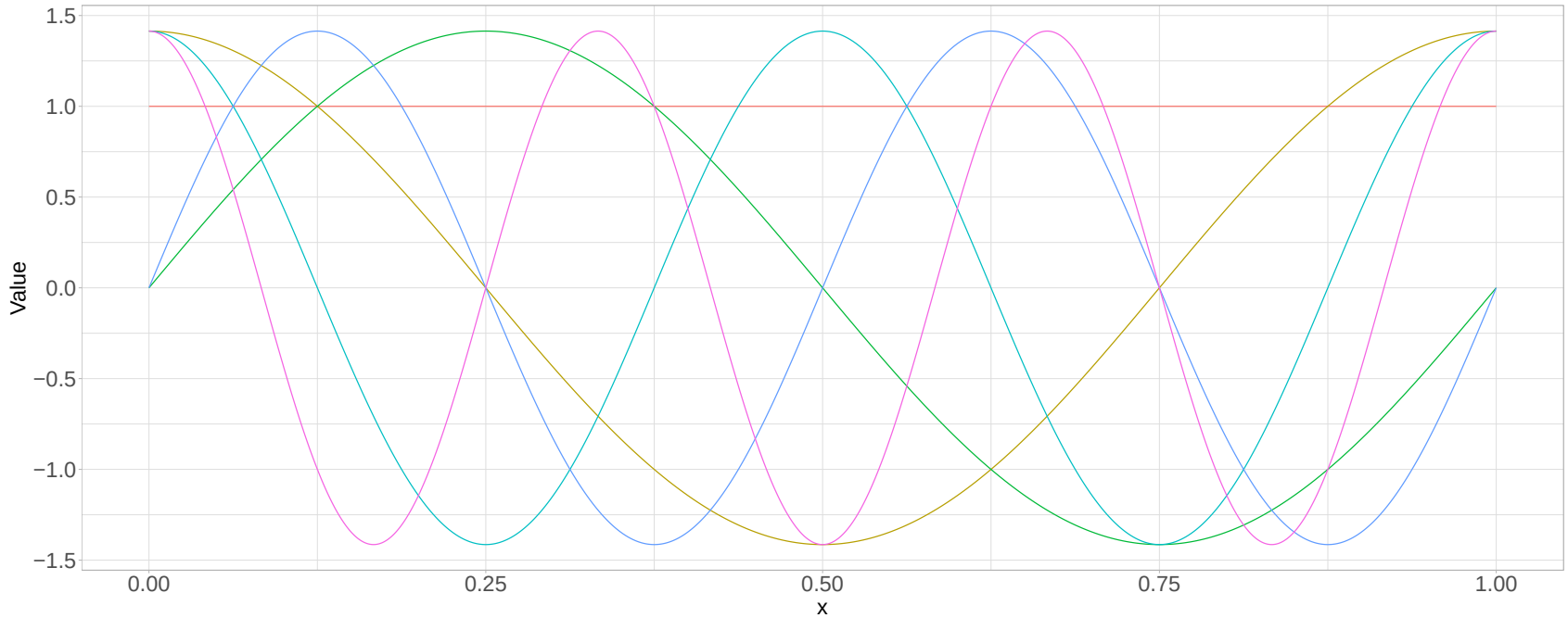
where $\phi_j(t)$ is the j^{th} basis function of the expansion and $c_{i,j}$ is the corresponding coefficient. We truncate the basis at L to:

- make the function smoother
- replace the original curves $x_i(t)$ with a smaller collection of $c_{n,m}$

Basis Functions

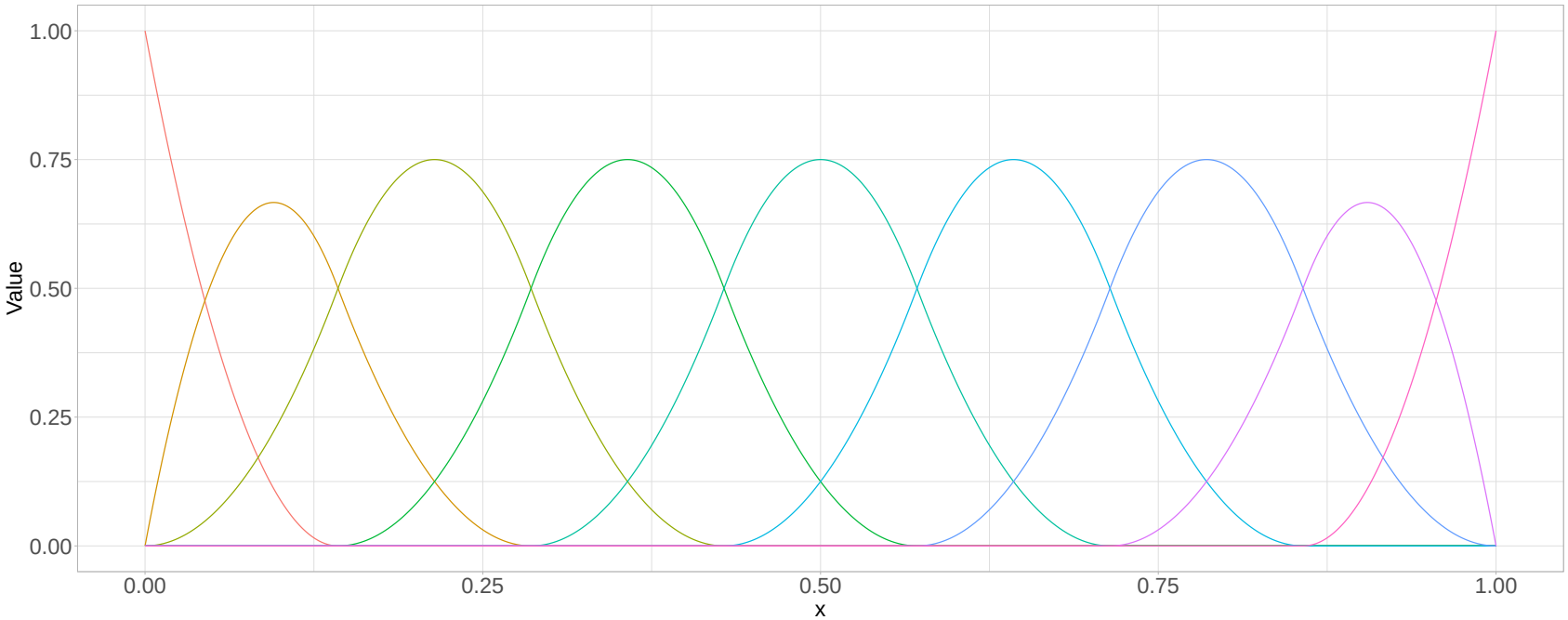
Fourier Basis Functions are elements of the set:

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



Basis Functions

B-spline Basis Functions are piece-wise polynomial functions defined by an order and a set of knots.



Trade Off between Bias and Variance

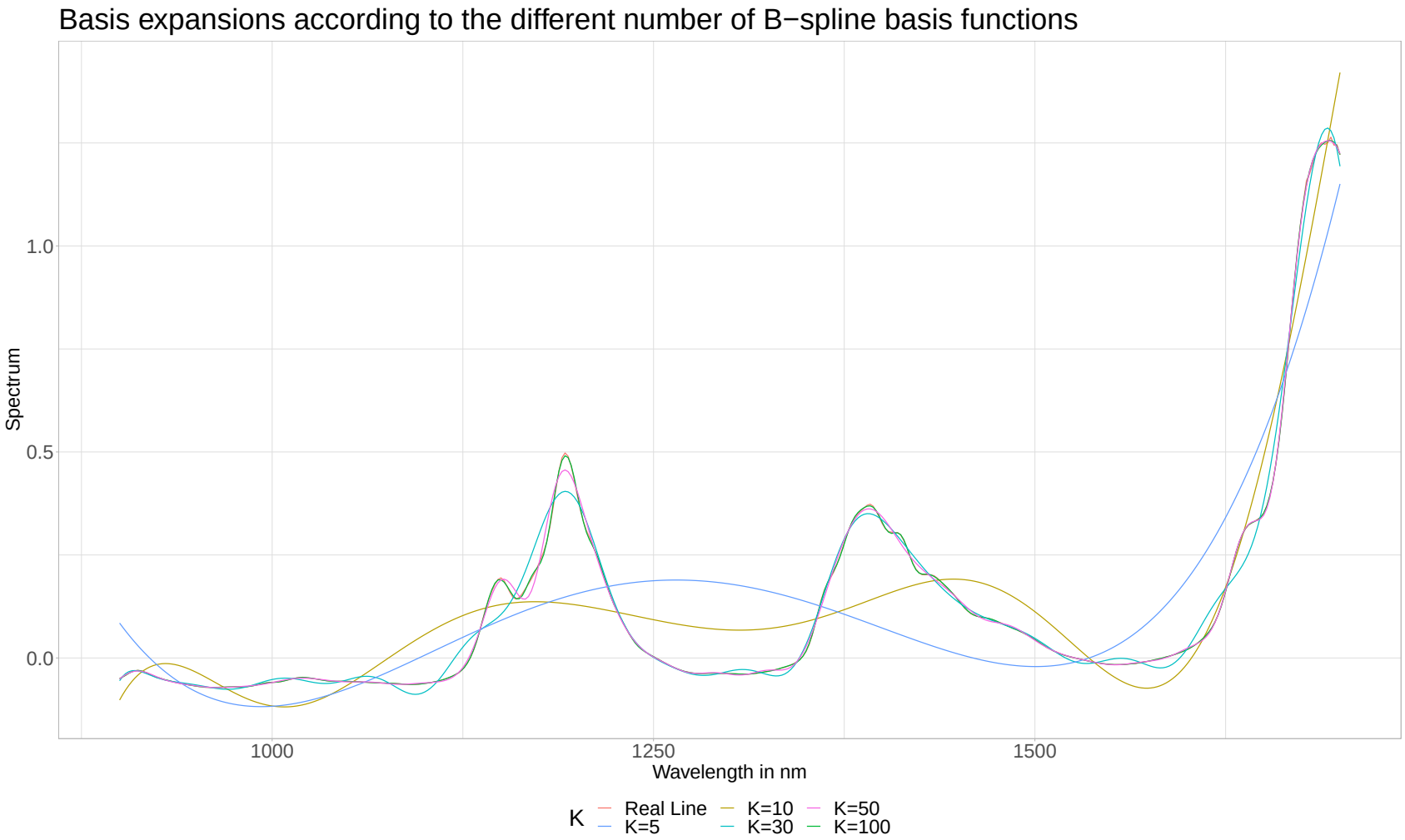
How do we choose the number L of basis functions?

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

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

- The larger L, the better the fit to the data, but also more fitting noise
- If L 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 $\{\phi_i(t) \mid i \in \mathcal{I}\}$ be a basis leading to the following representation

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

Estimation via Basis Representation

We can transform the data generating process into:

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

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

▸ Equation with Approximated Functions

Estimation via Basis Representation

Truncating the functional basis allows us to estimate coefficients using **Multivariate Regression** leading to an estimated coefficient vector $\hat{c} \in \mathbb{R}^L$ and an estimated coefficient function $\hat{\beta}_L(t)$:

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

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 $(\psi_j(t))_{j \in \mathcal{L}}$ used for the observations
- The truncation parameter for 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

Simulation Setup

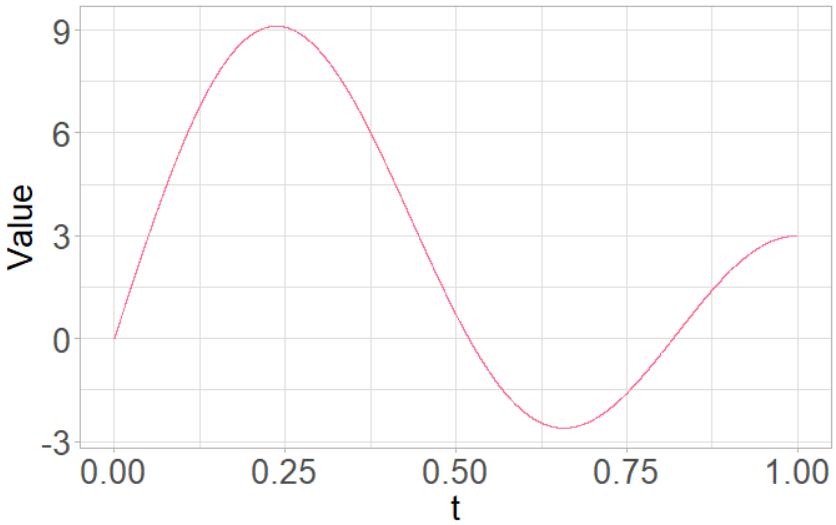
Use the **Gasoline Dataset** (NIR-spectroscopy, 60×401) to generate **Similar Curves**:

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

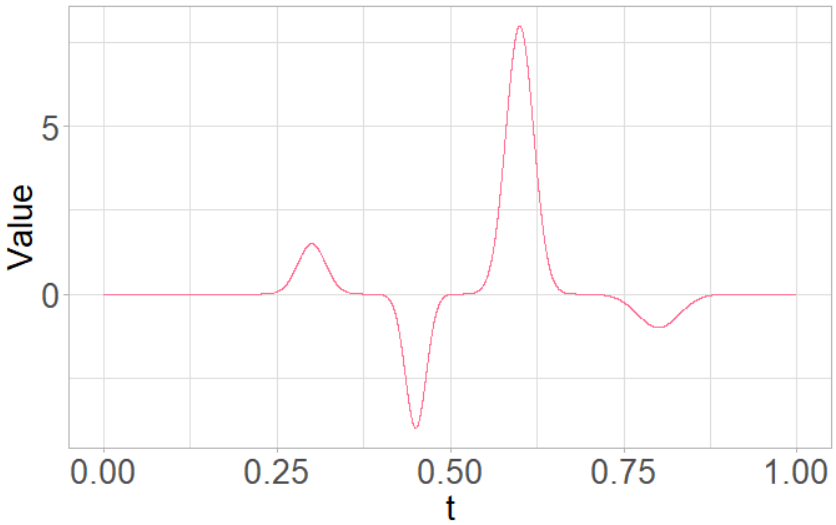
- $\tilde{\xi}_j \sim \mathcal{N}(0, \hat{\lambda}_j)$ and $\tilde{\xi}_j \perp\!\!\!\perp \tilde{\xi}_k$ for $j \neq k$
- Simplification: the ξ_j do not follow a normal distribution
- $\tilde{X}(\omega)(t)$, $\hat{\mu}(t)$ and $\hat{\nu}_j(t)$ are approximated as vectors in $\mathbb{R}^{401}$

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.

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

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

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

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

Simulation - Interpretation of Results

Basis Expansion Regression

- Smooth function requires smaller number of n_{basis} and vice versa
- Setup with higher noise requires smoother function

Performs better on bumpy function with low noise.

Functional Principal Component Regression

- Two Functional-PC enough to explain variation
- Results quite similar, but bspline setup better for smooth function with noisy response

Performs better in the noisy setup with the smooth function.

▸ Basis Expansion Results ▸ FPCR Results

Application Setup

Use insights from the simulation study to **predict the Octane Ratings**.

- Similar setup, but relying on the initial 60 spectral curves
- Validation set approach: Scores of test data needs to be estimated by the training data
- Report results by **IMSE** for the evaluated best model specifications

Further Reading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Kokoszka, Piotr and Matthew Reimherr (Aug. 2017). *Introduction to Functional Data Analysis*. Englisch. 1st ed. Boca Raton: Chapman and Hall/CRC. ISBN: 978-1-4987-4634-2.


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Ramsay, James and B. W. Silverman (2005). *Functional Data Analysis*. en. 2nd ed. Springer Series in Statistics. New York: Springer-Verlag. ISBN: 978-0-387-40080-8. DOI: 10.1007/b98888. URL: https://www.springer.com/de/book/9780387400808 (visited on 10/23/2021).


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

Estimation with Approximated Functions

$$
\begin{aligned}
Y(\omega) &= \alpha + \int_0^1 \beta(s)X(\omega)(s)\mathrm{d}s + \epsilon(\omega) \\
&= \alpha + \int_0^1 \left[\left(\sum_{j\in\mathcal{I}} c_j \phi_j(s) \right) \left(\sum_{k\in\mathcal{L}} d_k(\omega)\psi_k(s) \right) \right] \mathrm{d}s + \epsilon(\omega) \\
&= \alpha + \sum_{j\in\mathcal{I}} \left[c_j \sum_{k\in\mathcal{L}} d_k(\omega) \int_0^1 \phi_j(s)\psi_k(s)\mathrm{d}s \right] + \epsilon(\omega) \\
&= \alpha + \sum_{j\in\mathcal{I}} \left[c_j \sum_{k\in\mathcal{L}} Z_{j,k}(\omega) \right] + \epsilon(\omega) \\
&\approx \alpha + \sum_{j=1}^{L} \left[c_j \sum_{k=1}^{K} Z_{j,k}(\omega) \right] + \epsilon(\omega) = \alpha + \sum_{j=1}^{L} \left[c_j \tilde{Z}_j^K(\omega) \right] + \epsilon(\omega)
\end{aligned}
$$

▸ Equation without Approximated Functions

Simulation Results - bspline basis expansion

f_1, Y_1	f_1, Y_2	f_2, Y_1	f_2, Y_2	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

Results

Simulation Results - Fourier basis expansion

f_1, Y_1	f_1, Y_2	f_2, Y_1	f_2, Y_2	n_basis
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

▸ Results

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

f_1, Y_1	f_1, Y_2	f_2, Y_1	f_2, Y_2	expl. var	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

▸ Results

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

f_1, Y_1	f_1, Y_2	f_2, Y_1	f_2, Y_2	expl. var	n_basis
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

▸ Results