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 (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

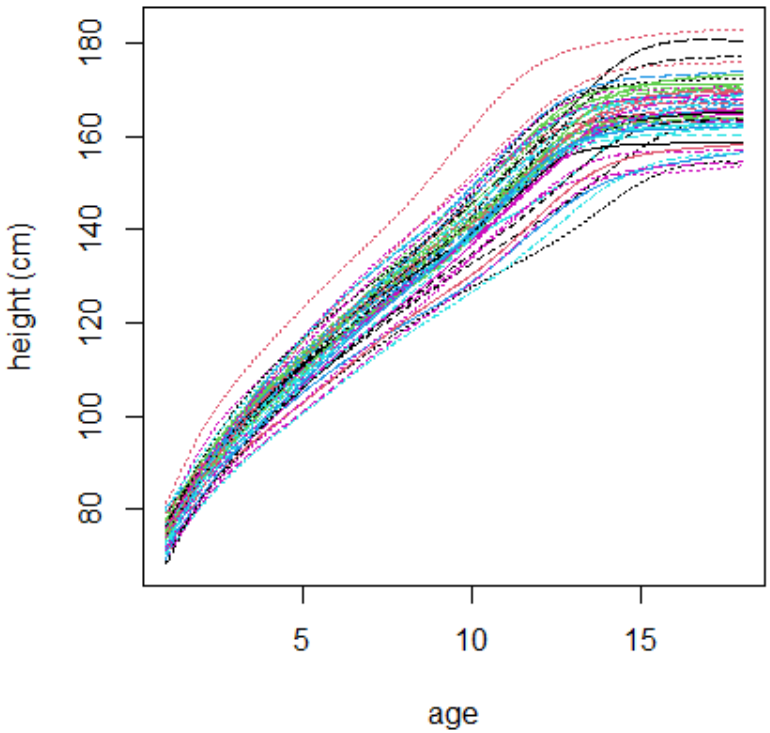
Let $\mathbb{E}$ be the index set and this can be described as

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

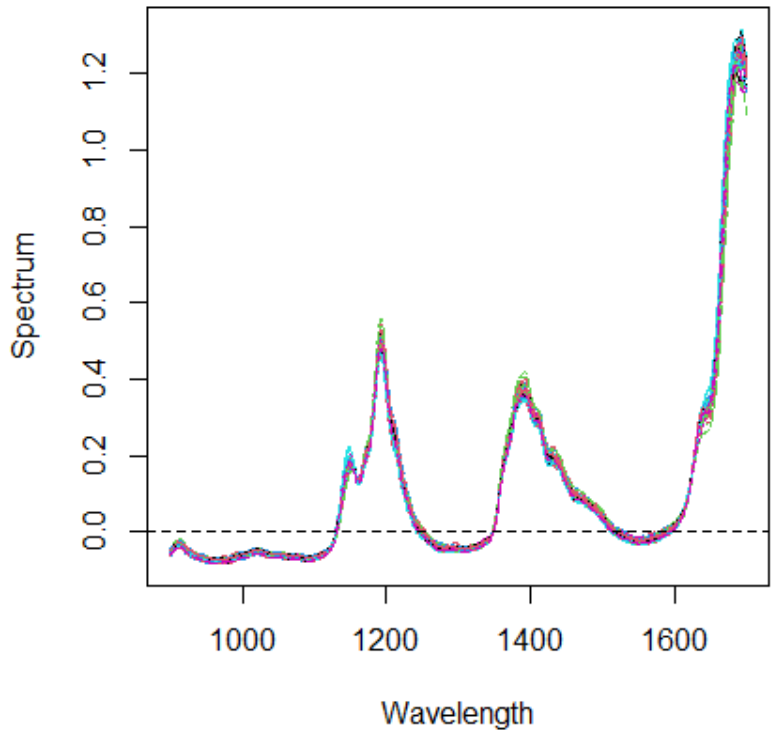
where $X(t, \cdot)$ is $\mathcal{F}$-measurable function on the sample space Ω.

- 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}

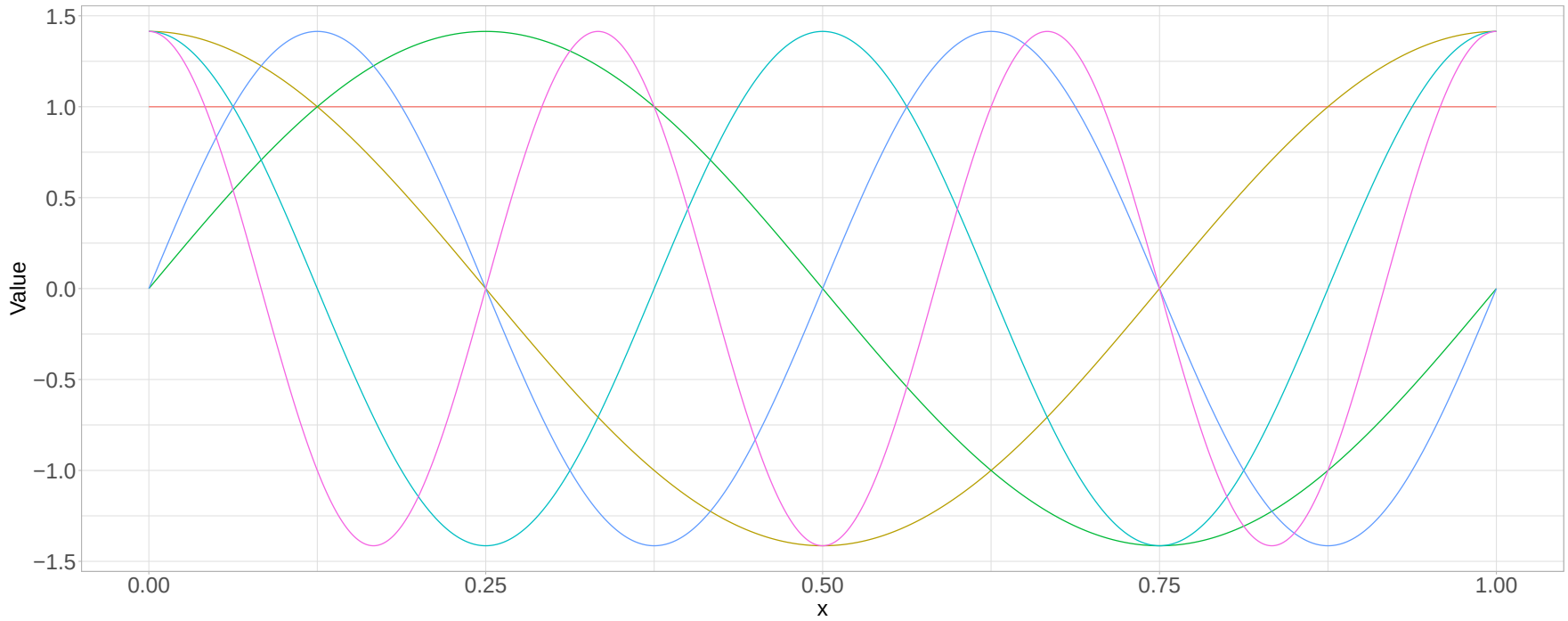
Two Typical Types of Basis Function

Fourier Basis Function is an element of the set:

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

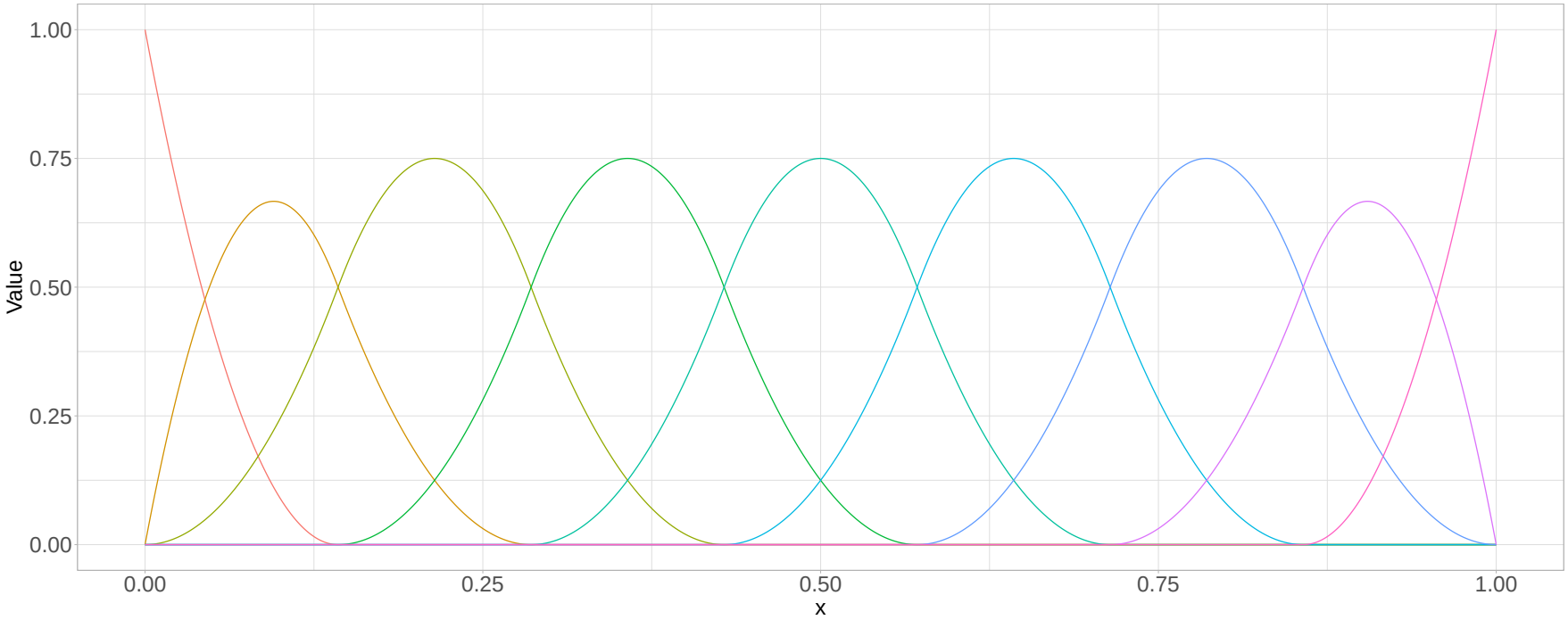
B-spline Basis Function is a polynomial function defined by order and knots.

Plots of Basis Functions



Fourier basis functions

Plots of Basis Functions



Bspline basis functions

Trade Off between Bias and Variance

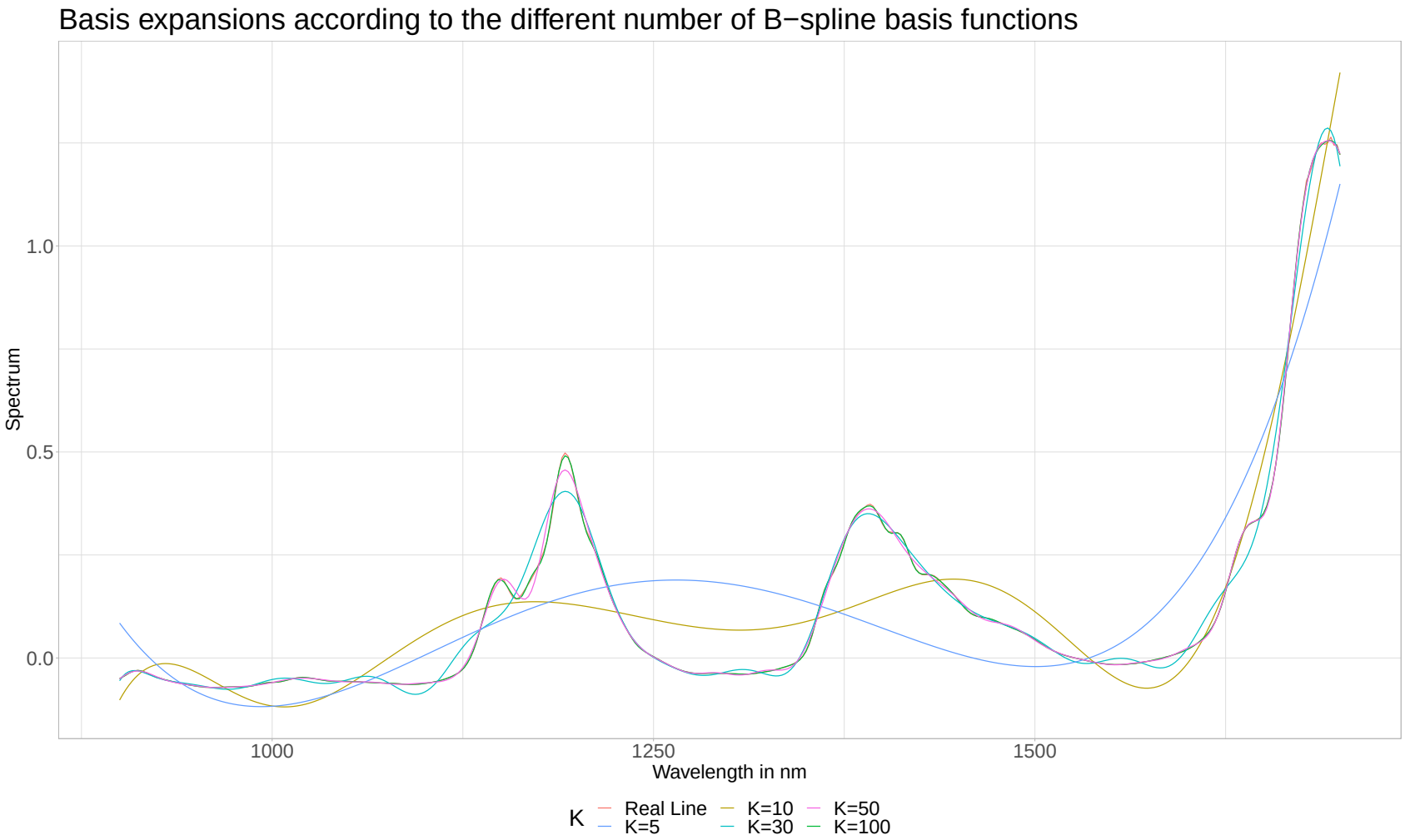
How do we choose the number K of basis functions?

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

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

- 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:

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

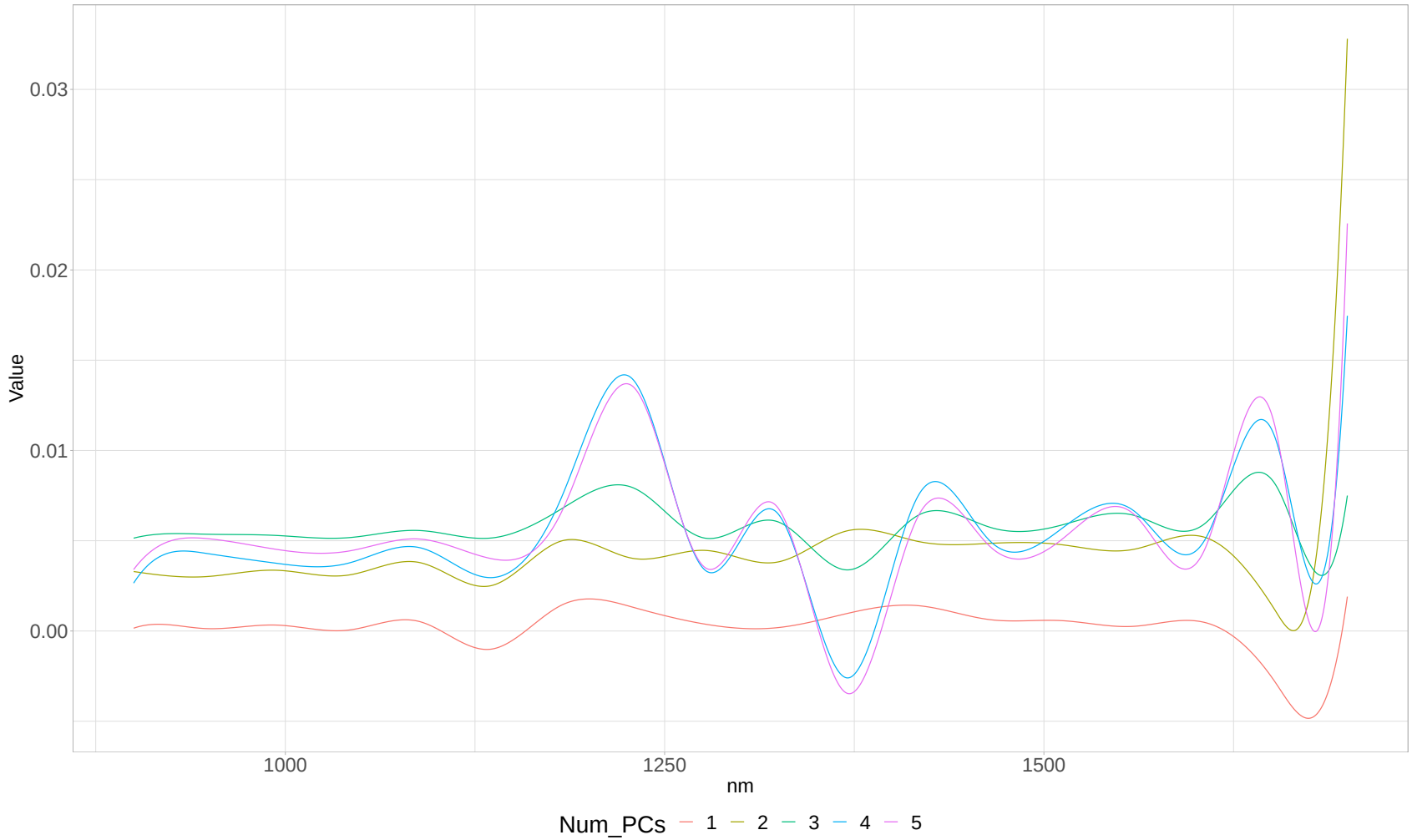
The $\{\hat{\nu}_i(s) \mid i \in \mathcal{I}\}$ are called **Functional Principal Components** and can serve as a basis for representing the original curves.

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

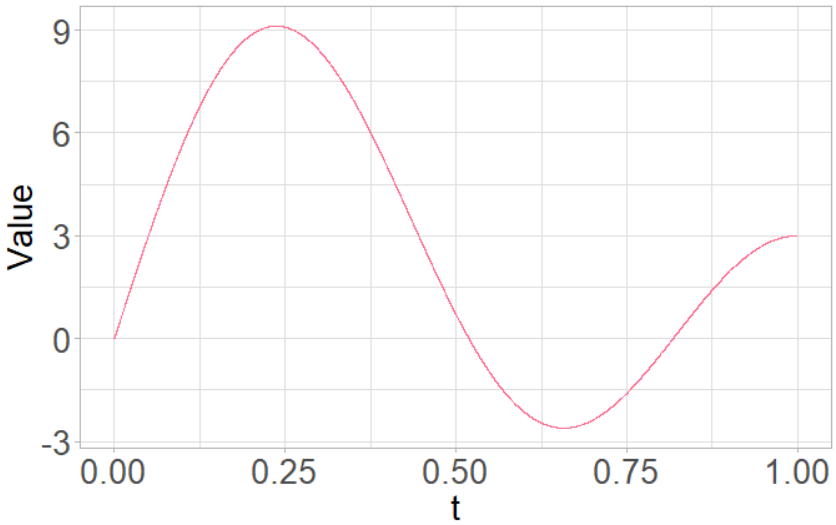
- Use the **Gasoline Dataset** (NIR-spectroscopy, 60×401) to predict octane ratings.
- Generate **similar curves** from gasoline dataset:

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

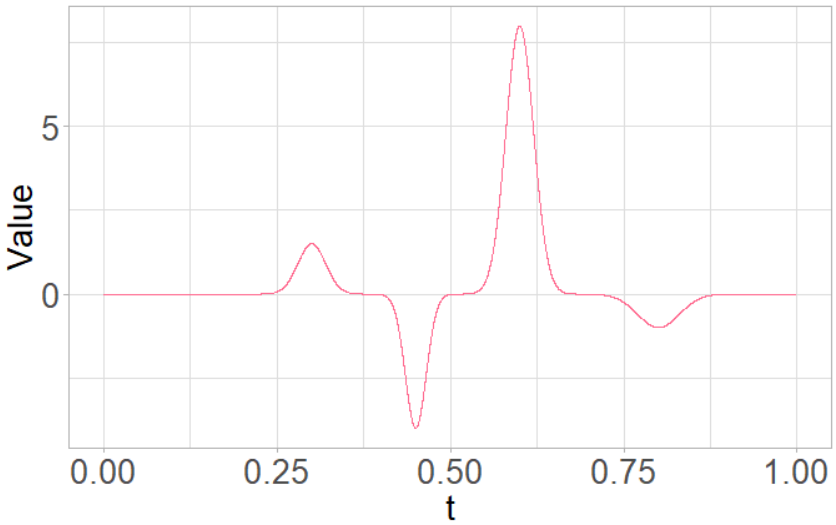
- $\tilde{\xi}_j \sim \mathcal{N}(0, \hat{\lambda}_j)$ and $\tilde{\xi}_j \perp\!\!\!\perp \tilde{\xi}_k$ for $j \neq k$
- Simplification: the ξ_j do not follow a normal
- $\tilde{X}(\omega)(t)$, $\hat{\mu}(t)$ and $\hat{\nu}_j(t)$ are approximated as vectors in $\mathbb{R}^{401}$.

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

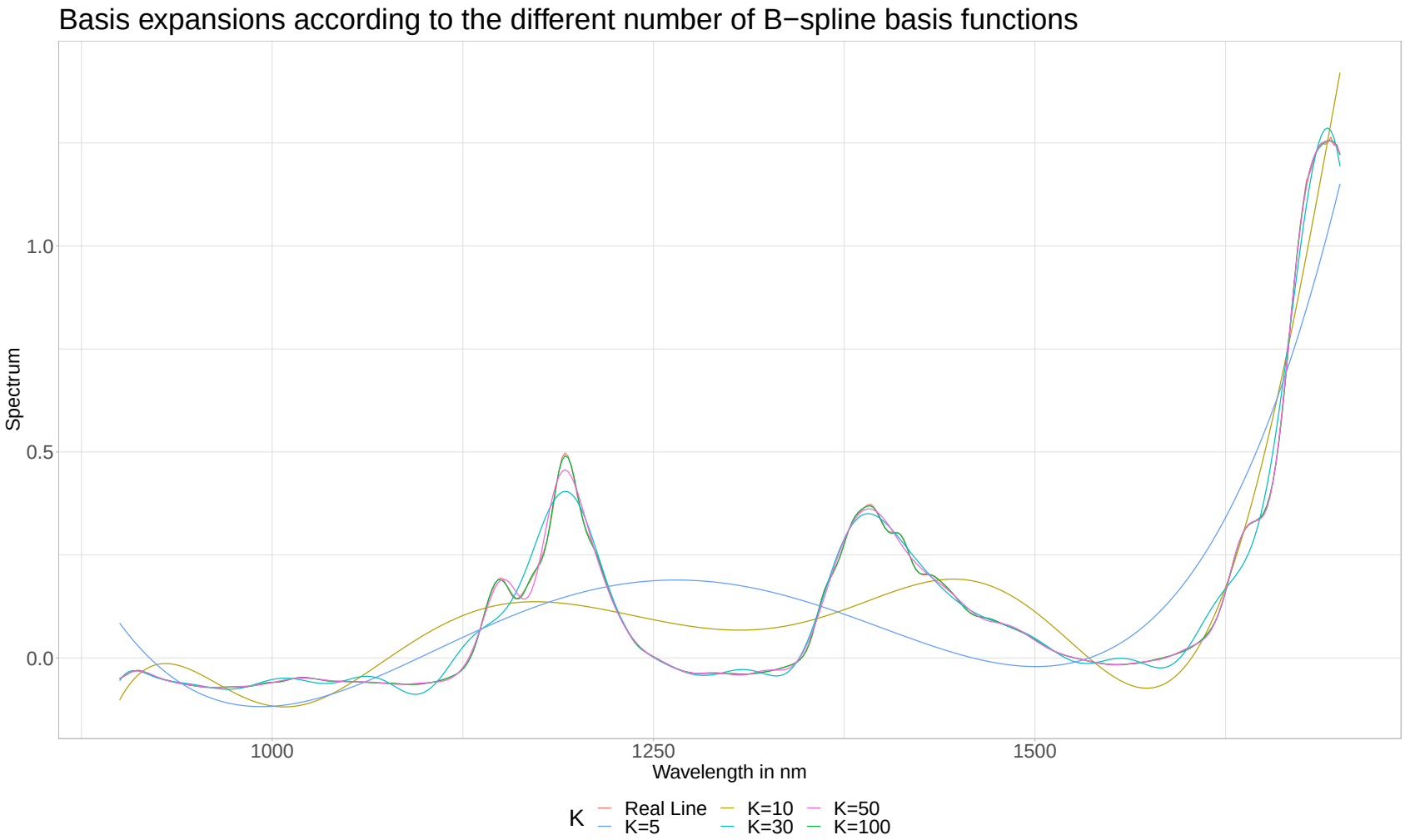
$$Y_{1,f} = \langle NIR, f \rangle + Z \left(\frac{var(\langle NIR, f \rangle)}{0.9} - var(\langle NIR, f \rangle) \right)$$

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

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 Results - bspline

f1_e1_spline	f1_e2_spline	f2_e1_spline	f2_e2_spline	n_basis
2.13178119016857	71.7099603226115	0.608171495504618	1.53453412563582	4
2.00756061672648	71.9395214288329	0.342736147598609	1.29059813220677	5
1.99374215191544	72.2563479644725	0.245623228181924	1.20138156565603	6
2.03648199621352	73.7857088138923	0.279709073157873	1.24948462939122	7
2.18614795862507	79.0485254545422	0.104397806306425	1.145842683177	8
2.05113790304629	74.1783834857012	0.0355899940503619	1.02172959116332	9
2.10522981230773	76.1883552769234	0.029691294210754	1.03929073546751	10
2.1011969989178	76.4030798206724	0.0296057602994908	1.04246508005367	11
2.38150697658292	86.1706579685565	0.0369986801764011	1.18191116948046	12
2.21136870222925	80.6207607207599	0.0363026864816967	1.10242516644568	13
2.44947712911835	87.6976578759761	0.0380185616636571	1.21257716080672	14
2.28870905624113	83.4755186453129	0.0315198808793299	1.13630733462095	15
2.5490614406393	93.593040512565	0.0351718970102256	1.26520057279256	16
2.55139454545527	93.3074090320499	0.0352440364348144	1.26610962599564	17
2.75160520792553	100.556190093422	0.0380316879790874	1.3620304183365	18
3.02429148497643	109.987580398216	0.0409879625688711	1.4813467852555	19
3.42548075922108	122.395980857659	0.0471595536208038	1.68537882583396	20
3.63355571510069	132.077208928751	0.0490939239286374	1.7750377827367	21
5.93680459997264	209.128064205703	0.0779161032701813	2.86105576687348	22
9.63325470698287	339.676032195418	0.126422677097386	4.65363116820157	23
15.2728939666428	545.827184915647	0.200212312881423	7.22652606521015	24
13.9781506322669	495.957265678323	0.184269309019229	6.6968929082163	25

Simulation Results - bspline

f1_e1_spline	f1_e2_spline	f2_e1_spline	f2_e2_spline	n_basis
2.02918344408687	72.0085477229407	0.511999648510189	1.47468049635309	3
2.0220366421201	72.60172284215	0.16157756089415	1.13746697354709	5
2.0354924731897	73.1836346250812	0.0293072016650537	0.990682620987463	7
2.06199840536677	73.9631412481736	0.0290190767234641	0.999385186246351	9
2.08808310984254	75.0920660376146	0.0290873388349217	1.01393568534507	11
2.09974789215127	75.9422236701681	0.0294100223429063	1.02909474969485	13
2.1086767501285	76.7123085769457	0.0298036585996321	1.03713735705978	15
2.13013296583489	77.4907530428231	0.0300236821233963	1.03980406503428	17
2.15348157839283	78.3942553410957	0.030307463717998	1.0508902800978	19
2.17750745519215	79.2057575714294	0.0306501467540424	1.06172373892826	21
2.20581113466118	80.3800790338639	0.0309985992677207	1.07695651700849	23
2.23717951397715	81.5089652049561	0.0314869147262958	1.09052842774153	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