Lecture 0: Overview of Function Spaces and Operator Theory

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PhD course
An Introduction to Functional Data Analysis: Theory and Practice

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Outline

1. Introduction
2. Function Spaces
   - Metric spaces, vector and normed spaces
   - Banach and L^p spaces
   - Inner product and Hilbert spaces
3. Linear Operators and Functionals
   - Linear and Integral operators
   - Spectral Decomposition and Karhunen-Loeve expansion

Main Reference: Chapters 2 and 3 in H&E[1]

[1] Hsing & Eubank, 2015: Theoretical Foundations of FDA, with an Introduction to Linear Operators. *Wiley Series in Probability & Statistics.*

Motivation

A first "loose" definition

Functional Data can be viewed as a collection of sample paths from a stochastic process (or processes) on the index set T

Therefore

- data are functions that might have various properties (continuity, square integrability, . . .) with probability 1
- an understanding of function spaces is an **essential** first step in dealing with functional data

Purpose of Lecture 0

Overarching Purpose

Present the function space theory that we perceive to be most relevant for Functional Data Analysis (FDA) $\rightarrow$ subjective choice!

Precise plan:

1. Function Spaces
   - metric spaces, vector and normed spaces
   - Banach and L^p spaces
   - inner product and Hilbert spaces
2. Linear Operators and Functionals
   - Linear and Integral operators
   - Spectral Decomposition and Karhunen-Loeve expansion

Metric Spaces

Metric spaces represent a natural topological abstraction of $\mathbb{R}^p$ that is suitable to the purposes of FDA

Definition 1: Metric Space

A *metric* on a set $\mathbb{M}$ is a function $d : \mathbb{M} \times \mathbb{M} \to \mathbb{R}$ that satisfies

1. $d(x_1, x_2) \geq 0$ (positivity)
2. $d(x_1, x_2) = 0$ if $x_1 = x_2$ (distance to itself)
3. $d(x_1, x_2) = d(x_2, x_1)$ (simmetry)
4. $d(x_1, x_3) \leq d(x_1, x_2) + d(x_2, x_3)$ (triangular inequality)

for $x_1, x_2, x_3 \in \mathbb{M}$. The pair $(\mathbb{M}, d)$ is then defined *metric space*

Example of a Metric Space

Example 2.1.3 in H&E

A somewhat "exotic" example of a metric space is $C\,[0,1]$, the set of continuous functions[a] on $[0,1]$. The sup metric is well-defined as

$$d(f,g) = \sup\left\{|f(t) - g(t)| : t \in [0,1]\right\}$$

for $f, g \in C\,[0,1]$. Conditions 1-4 in Definition 1 can be easily verified for this case (try!)

[a] Continuous functions defined on a closed interval are uniformly continuous.

Vector Spaces

The concept of **vector spaces** provides the addition of an algebraic structure to metric spaces, which will be useful in the following lectures

Definition 2: Vector Space

A vector space $\mathbb{V}$ is a set of elements (referred to as vectors) for which two operations have been defined: addition and scalar multiplication

- given two vectors $v_1, v_2 \in \mathbb{V}$, *addition* returns another vector in $\mathbb{V}$ denoted $v_1 + v_2$
- given a vector $v \in \mathbb{V}$ and a scalar $a \in \mathbb{R}$, *scalar multiplication* returns a vector in $\mathbb{V}$ denoted by av

Properties of the Addition and Multiplication

1. $v_1 + v_2 = v_2 + v_1$
2. $(v_1 + v_2) + v_3 = v_1 + (v_2 + v_3)$, and $a_1(a_2 v) = (a_1 a_2)v$
3. $a(v_1 + v_2) = av_1 + av_2$, and $(a_1 + a_2)v = a_1 v + a_2 v$
4. $1v = v$
5. $\exists!$ element 0 with the property that $v + 0 = v$ for all $v \in \mathbb{V}$
6. $\forall v \in \mathbb{V}$, $\exists$ element $(-v) \in \mathbb{V}$ such that $v + (-v) = 0$

Definition 3: Span

If $A \subset \mathbb{V}$ is a subset of a vector space, $span(A)$ is the **smallest subspace** (i.e., the intersection of all subspaces) in $\mathbb{V}$ including all elements of A. Differently from A, $span(A)$ is a subspace as it has the same algebraic structure as $\mathbb{V}$, since it includes the elements of A together with all their finite dimensional linear combinations.

Basis for Vector Spaces

Linearly independent collections

Let $\mathbb{V}$ be a vector space, and $B = \{v_1, \dots, v_k\} \subset \mathbb{V}$ for some finite positive integer k. The collection of elements B is *linearly independent* if $\sum_{i=1}^{k} a_i v_i = 0 \Rightarrow a_i = 0 \ \forall \ i = 1, \dots, k$.

Definition 4: Basis

If $B = \{v_1, \dots, v_k\}$ is a linearly independent subset of the vector space $\mathbb{V}$ and $span(B) = \mathbb{V}$, then B is a *basis* for $\mathbb{V}$.

Note that, if $\{v_1, \dots, v_k\} \subset \mathbb{V}$ is a basis and $v \in \mathbb{V}$ is any element of the vector space, then there exists coefficients $b_1, \dots, b_k$ such that

$$v = \sum_{i=1}^{k} b_i v_i$$

Normed Vector Space

Adding a measure of "distance" called a *norm* to a vector space allows to merge the concept of metric and vector spaces.

Definition 5: Norm

Let $\mathbb{V}$ be a vector space. A norm on $\mathbb{V}$ is a function $||\cdot|| : \mathbb{V} \to \mathbb{R}$ such that

1. $||v|| \geq 0$; $||v|| = 0 \Leftrightarrow v = 0$
2. $||av|| = |a|||v||$
3. $||v_1 + v_2|| \leq ||v_1|| + ||v_2||$

$\forall\ v, v_1, v_2 \in \mathbb{V}$ and $a \in \mathbb{R}$. $\mathbb{V}$ is then a *normed vector space.*

Remark: if $\mathbb{V}$ is a normed vector space with norm $||\cdot||$, then *it is also a metric space*, with respect to the *norm-induced metric:*

$$d(x, y) := ||x - y|| \text{ for } x, y, \in \mathbb{V}.$$

Banach and L^p Spaces

Many normed vector spaces are complete[2], a special subset being:

Definition 6: Banach spaces

A *Banach space* is a normed vector space which is complete under the norm-induced metric.

The following group of Banach spaces are quite important for FDA:

Definition 7: L^p spaces

For $(E, \mathcal{B}, \mu)$ measure space and $p \in [1, \infty)$, let $L^p(E, \mathcal{B}, \mu)$ be the collection of measurable functions f on E s.t. $\int_E |f|^p d\mu < \infty$. $L^p(E, \mathcal{B}, \mu)$ is then a Banach space wrt the natural norm:

$$||f||_p = \left(\int_E |f|^p d\mu \right)^{1/p}$$

[2] A metric space $(\mathbb{M}, d)$ is *complete* if every Cauchy sequence is convergent.

L^p Spaces cnt'd

Definition 7: L^p spaces cnt'd

The collection of measurable functions f on E that are finite a.e. wrt μ is denoted by $L^\infty(E, \mathcal{B}, \mu)$, which is a Banach space with respect to the natural norm

$$||f||_\infty = \operatorname*{esssup}_{s \in E} |f(s)| = \inf \{x \in \mathbb{R} : \mu(s : |f(s)| > x) = 0\}$$

Warning: imprecise notation! I have assumed that $|| \cdot ||_p$ defined a norm, but the property $||f||_p = 0 \Leftrightarrow f = 0$ is only true a.e. wrt μ. However, the following convention is generally adopted, that *functions differing on a set of μ measure 0 are the same function*

$$f \sim g \text{ if } \mu \{x : f(x) \neq g(x)\} = 0,$$

and the L^p spaces introduced before are *identified with their quotient spaces of equivalence classes.*

The easiest and most common situation

We have been so far very general, but remember that for the purposes of FDA the following choices will typically apply:

- $E = [0, 1]$ (or some closed $T \subset \mathbb{R}$)
- $\mathcal{B}$ is the Borel σ-field of $[0, 1]$
- μ is the Lebesgue measure

For easiness of notation, we will refer to the L^p space corresponding to the above choices simply as $L^p([0, 1])$, or $L^p(T)$ for $T \subset \mathbb{R}$.

Inner product

Definition 8: Inner product

A function $\langle \cdot, \cdot \rangle$ on a vector space $\mathbb{V}$ is called an inner product if it satisfies

1. $\langle v, v \rangle \geq 0$
2. $\langle v, v \rangle = 0$ if $v = 0$
3. $\langle v_1, v_2 \rangle = \langle v_2, v_1 \rangle$
4. $\langle a_1 v_1 + a_2 v_2, v \rangle = a_1 \langle v_1, v \rangle + a_2 \langle v_2, v \rangle$

$\forall\ v, v_1, v_2 \in \mathbb{V}$, and $a_1, a_2 \in \mathbb{R}$.

The inner product provides the framework needed to extend to abstract settings the *orthogonality* concept of Euclidean spaces:

Orthogonality

$v_1, v_2 \in \mathbb{V}$ are *orthogonal* if and only if $\langle v_1, v_2 \rangle = 0$

Useful properties of the inner product

A vector space $\mathbb{V}$ equipped with an inner product is called an *inner-product space*.
The inner-product space $\mathbb{V}$ with inner product $\langle \cdot, \cdot \rangle$ is a normed space wrt the norm $|| \cdot ||$ defined by $||v|| = \sqrt{\langle v, v \rangle}$ for $v \in \mathbb{V}$.

Definition 9: Hilbert Space

A complete inner-product space is called a *Hilbert space.*

An orthonormal sequence[3] $\{e_n\}$ in a Hilbert space $\mathbb{H}$ is called an *orthonormal basis* if *span* $\{e_n\} = \mathbb{H}$. $\forall x \in \mathbb{H}$ it then holds:

$$x = \sum_{j=1}^{\infty} \langle x, e_j \rangle e_j \quad \text{and} \quad ||x||^2 = \sum_{j=1}^{\infty} \langle x, e_j \rangle^2 \quad \text{(Fourier expansion)}$$

[3] See Definition 2.4.8 and Theorem 2.4.10 at page 33-34 of H&E

The special case of L^2

Among all Banach L^p spaces, the only one that is also Hilbert is L^2, equipped with the inner product:

$$\langle f_1, f_2 \rangle = \int_E f_1 f_2 d\mu \quad \text{for} \quad f_1, f_2 \in E$$

The following result holds

Theorem

L^2 is a *separable*[a] Hilbert space wrt the Fourier bases (see Theorem 2.4.18 at page 36 of H&E).

[a] An Hilbert space that admits an orthonormal basis.

Remark: the rest of the theory in Chapter 2 of H&E is very interesting, but we have no time to go into it! :)

Linear Operators

Remark: a vector space that does not possess a finite dimensional basis is *infinite dimensional*, and a proper definition of a "basis" entails considerable complications. Therefore, we focus on the easier case of *orthonormal bases for separable Hilbert spaces*.

Definition 10: Linear Operator

Let $\mathbb{V}_1, \mathbb{V}_2$ vector spaces. A mapping $\mathcal{T} : \mathbb{V}_1 \to \mathbb{V}_2$ is said to be a *linear operator* if $\mathcal{T}(a_1 v_1 + a_2 v_2) = a_1 \mathcal{T}(v_1) + a_2 \mathcal{T}(v_2)$ for all $a_1, a_2 \in \mathbb{R}$ and $v_1, v_2 \in \mathbb{V}$

For $\mathbb{X}_1, \mathbb{X}_2$ normed vector spaces with norms $||\cdot||_1$ and $||\cdot||_2$, resp, the linear operator $\mathcal{T} : \mathbb{X}_1 \to \mathbb{X}_2$ is *bounded* if there exists a finite constant $C > 0$ such that $||\mathcal{T}x||_2 \leq C||x||_1$ for all $x \in \mathbb{X}_1$.

Theorem: linear operator + bounded $\Rightarrow$ *uniformly continuous*

Integral Operators in the L^2 case

Important class of linear operators in L^2 are *integral operators*

Integral Operator

$\Psi : L^2[0,1] \to L^2[0,1]$ induced by $\psi(\cdot,\cdot)$ such that

$\Psi(f)(t) = \int \psi(t,s) f(s) ds$ where $\psi : [0,1] \times [0,1] \to \mathbb{R}$ continuous

Assume that $\int\int |\psi(s,t)|^2 ds dt < \infty$, then Ψ satisfies

- $\langle \Psi(f), g \rangle = \langle f, \Psi(g) \rangle \ \forall \ f, g \in L^2[0,1]$ (symmetric)
- $\langle \Psi(f), f \rangle \geq 0 \ \forall \ f \in L^2[0,1]$ (positive definite)
- $\Psi(\cdot) = \sum_{k \geq 1} \lambda_k \langle \cdot, f_k \rangle g_k$, where $\{f_k\}$ and $\{g_k\}$ are two orthonormal bases in $L^2[0,1]$ and $\lambda_n \overset{n\to\infty}{\to} 0$ (compact)

Spectral Decomposition

One crucial result for the extension of Principal Component Analysis (PCA) to functional data connects to the spectral decomposition of operators:

Mercer's Theorem

Let $\psi(\cdot,\cdot)$ be symmetric and positive definite, and let Ψ be the corresponding integral operator. If (λ_i, e_i) are the eigenvalue and eigenfunction pairs of Ψ, then $\psi(\cdot,\cdot)$ can be written as

$$\psi(s,t) = \sum_{j=1}^{\infty} \lambda_j e_j(s) e_j(t), \qquad \forall s,t$$

and the above series converges absolutely and uniformly.

Karhunen-Loeve expansion

Assume Ψ symmetric, positive definite, and compact operator with finite norm. Then Mercer's theorem implies that

$$\Psi(\cdot) = \sum_{j=1}^{\infty} \lambda_j \langle \cdot, e_j \rangle e_j$$

where the λ_j's are the eigenvalues and e_j's are the eigenfunctions of Ψ, which means that $\Psi(e_j) = \lambda_j e_j$ and $\lambda_1 \geq \lambda_2 \geq \ldots 0$

Remark: first intuition about fPCA! This result allows writing elements of the functional space as basis expansions wrt to the eigenfunctions of a very special integral operator, which we will discover (later) being the covariance operator.

Summary

- Functional data are elements of infinite dimensional spaces!
- Soft introduction to the theory behind such spaces:
  - Metric, vector, and normed spaces
  - Basis expansions
  - Banach and L^p spaces
  - Hilbert spaces, and the case of L^2
  - Linear and Integral Operators
  - Spectral Decompositions
- From Lecture 1, the course will combine theory with practical applications! (this was very abstract, the rest will not be) But *the theory introduced here serves as ground* to understand some results which will be used.