Functional Data Analysis

Week 2.

Topics covered:

- Elements of Hilbert Spaces
- Random Elements on Function Space.
- Basic Inference on Function Space.

Starting point: We are given $X_1, \dots, X_N$ curves on the domain $[0,1]$.

Natural approach: Assume X_i is a realisation of $\{X_t : t \in [0,1]\}$

$\wr$

$X(t,\cdot)$ is a $\mathbb{R}$-value RV for each $t \in [0,1]$

Q: What's the relationship between $X(t,\cdot)$, $X(t',\cdot)$?

Alternative View: Assume that $X_1, \dots, X_N$ are indep samples of a "Function-Spaced" RV, i.e.

$(\Omega, \mathcal{F}, \mathbb{P})$

$$X_i \sim X,$$

$$X : \Omega \to H$$ which is measurable.

i.e. $X(\omega)$ is a random curve.

Which function space? In FDA take $L^2([0,1])$, which is a Hilbert space.

Recall: A vector space V is an inner product space with inner product $\langle \cdot, \cdot \rangle$ if

- $\langle x, y \rangle = \langle y, x \rangle$ for all $x \in V$, $y \in V$
- $\langle a x_1 + b x_2, y \rangle = a \langle x_1, y \rangle + b \langle x_2, y \rangle$
- $\langle x, x \rangle \geq 0$ and $\langle x, x \rangle = 0$ if and only if $x = 0$.

Ex. $(\mathbb{R}^d, \langle u, v \rangle = u \cdot v)$ is an IPS.

An inner product defines a norm

$$\|x\| = \sqrt{\langle x, x\rangle}$$

Ex. $\mathbb{R}^d$, $\|\cdot\|$ = length of vector.

<u>Def^n</u>: A <u>metric space</u> in which every Cauchy sequence has a limit is stb <u>complete</u>

$(x_n)_{n\in\mathbb{N}}$ is stb Cauchy if $\forall \varepsilon > 0$, $\exists N \in \mathbb{N}$ s.t. $\forall n, m \geq N$, $d(x_n, x_m) < \varepsilon$

<u>Def^n</u>: An inner product space which is also complete (wrt the norm induced by $\langle \cdot, \cdot \rangle$) is s.t.b a <u>HILBERT SPACE</u>.

Remark $(\mathbb{R}^d$ with $\langle \cdot, \cdot \rangle$ = dot product$)$ is a Hilbert Space.

<u>Ex 1</u>: The space ℓ^2: This is the set of all sequences

- $V = \{ x = (x_1, x_2, x_3, \dots) \text{ s.t. } \sum |x_i|^2 < \infty \}$

- Then V is a vector space under componentwise addition, i.e.

  - $x + y = (x_1 + y_1, x_2 + y_2, \dots)$

  and scalar multiplication.

- V is an inner product space under

$$\langle x, y \rangle = \sum_{i=1}^{\infty} x_i y_i$$

- In fact V is a Hilbert space.

Def: The space $L^2([0,1])$ is the collection of all Lebesgue measurable real-valued functions x defined on $[0,1]$ s.t.

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

- Addition: $(x+y)(t) = x(t) + y(t)$.

Scalar mult: $(\lambda x)(t) = \lambda x(t)$.

- The inner product:

$$\langle x, y\rangle = \int_0^1 x(t)y(t)\,dt.$$

- This induces a norm:

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

- $L^2([0,1])$ is a Hilbert space.

In this space, the Cauchy-Schwartz inequality looks like:

$$\langle x, y\rangle \leq \|x\|\,\|y\|.$$

$$\left|\int_0^1 x(t)y(t)\,dt\right| \leq \left(\int |x|^2(t)\,dt\right)^{\frac{1}{2}}\left(\int |y|^2(t)\,dt\right)^{\frac{1}{2}}$$

Ex $L^2(\mathbb{R}) = \{$ set of square integrable functions on $\mathbb{R}\}$, same inner product, it's a Hilbert space.

Note: $\forall\, x \in L^2(\mathbb{R})$ then x must decay in the tails.

One can define

$$L^2_\omega(\mathbb{R}) = \left\{ x : \int x(t)^2 \, \omega(t) \, dt < \infty \right\}$$

e.g. $\omega(t) = e^{-t^2/2}$.

Definition (Sobolev Space) Define $H^K([0,1])$ to be the functions in $L^2([0,1]$ whose (weak) derivatives up to order K are also in L^2.

This is a Hilbert space with inner product:

$$\langle x, y \rangle_{H^K} = \sum_{k=0}^{K} \int D^{(k)} x(t) \, D^{(k)} y(t) \, dt.$$

Eg. when $k=1$:

$$\langle x, y \rangle_{H^1} = \int_0^1 x(t) \, y(t) \, dt + \int Dx(t) \, Dy(t) \, dt$$

$$= \langle x, y \rangle + \langle Dx, Dy \rangle.$$

e.g. Consider $C[0,1]$ of all continuous functions on $[0,1]$. with

$$\|x\| = \sup_{t \in [0,1]} |x(t)|.$$

defines a normed space, in fact a Banach space.

<u>Recall</u>: $\{e_i : i \in I\}$ is an ORTHONORMAL SYSTEM if

- $\langle e_i, e_i \rangle = 1$
- $\langle e_i, e_j \rangle = 0$ if $i \neq j$.

<u>Def^{n}</u>: H is s.t.b. separable if there is a countable orthonormal system $\{e_1, e_2, \ldots\}$ s.t. $\forall x \in H$ I can write:

$$\boxed{x = \sum_{j=1}^{\infty} \underline{a_j} e_j} \quad (*)$$

In this case, $\{e_1, e_2, \ldots\}$ is s.t.b. an orthonormal basis. (ONB)

$$\hookrightarrow \lim_{J\to\infty} \left\| x - \sum_{j=1}^{J} a_j e_j \right\| = 0$$

$$\langle x, e_k \rangle = \left\langle e_k, \sum a_j e_j \right\rangle$$

$$= \sum a_j \langle e_k, e_j \rangle = a_k.$$

<u>So:</u>

$$x = \sum_{j=1}^{\infty} \langle x, e_j \rangle e_j$$

$$\|x\|^2 = \langle x, x \rangle = \left\langle \sum_{j=1}^{\infty} \langle x, e_j \rangle e_j, \sum_{k=1}^{\infty} \langle x, e_k \rangle e_k \right\rangle$$

$$= \sum_{j,k}^{\infty} \langle x, e_j \rangle \langle x, e_k \rangle \underbrace{\langle e_j, e_k \rangle}_{\delta_{jk}}$$

$$= \sum_{j=1}^{\infty} |\langle x, e_j \rangle|^2$$

PARSEVAL'S IDENTITY.

Focus on $L^2([0,1])$, Examples of ONB.

$e_1(t) = 1$, $\quad e_2(t) = \sqrt{2}\sin(2\pi t)$,

$e_3(t) = \sqrt{2}\cos(2\pi t)$

$e_4(t) = \sqrt{2}\sin(4\pi t)$

$\vdots$

- <u>One can check</u>: this is a ONB for $L^2([0,1])$

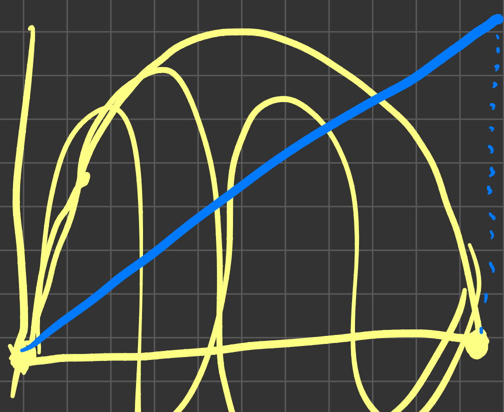
- <u>for example</u> $f_0, f_1, f_2, \ldots$

$f_0(t) = 1$, $\quad f_k(t) = \sqrt{2}\cos(\pi k t)$, $k \geq 1$

forms an ONB for $L^2([0,1])$.

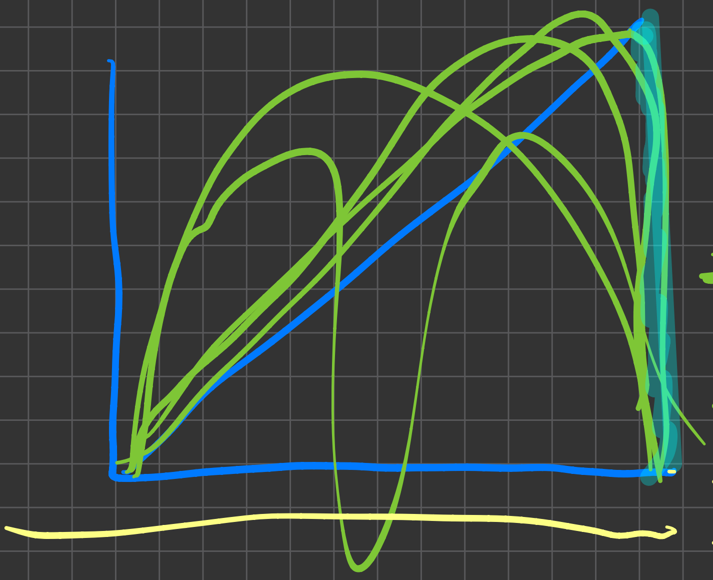
- <u>Also</u>: $g_1, g_2, \ldots$, $\quad g_k = \sin(k\pi t)$, $k \geq 1$

also an ONB for $L^2([0,1])$.



Consider $f(t) = t$.

$$\int_0^1 f^2(t)\,dt = \int_0^1 t^2\,dt = \frac{1}{3} < \infty$$



$$\| x - \sum \langle x, g_n \rangle g_n \| \Rightarrow \int | x - \sum \langle x, g_n \rangle g_n |^2 \, dt \to 0$$

Linear Functionals and Linear Operators on H.

- $\ell : H \to \mathbb{R}$ is a linear functional:

$$\ell(\alpha x + \beta y) = \alpha \ell(x) + \beta \ell(y), \quad \forall \alpha, \beta \in \mathbb{R}, \ \forall x, y \in H$$

- ℓ is s.t.b bounded if $\exists K > 0$ s.t.

$$|\ell(x)| \leq K \|x\|.$$

The smallest such K is called the norm of ℓ: $\|\ell\|$:

i.e.

$$\|\ell\| = \sup_{\|x\| = 1} |\ell(x)|$$

$$\ell_t(x) = x(t)$$

PROBE FUNCTIONS

Examples: Let $g \in H$, take $\ell_g(x) = \langle g, x \rangle$ $\forall x \in H$.

CHECK Bounded linear functional

$\|\ell\| = \|g\|$.

Thm (Riesz Representation Theorem)

If $\ell : H \to \mathbb{R}$ is a bounded linear fnl

then $\exists!\, g \in H$ s.t.

$$\ell(x) = \langle g, x \rangle \quad \forall x \in H.$$

A function $L : H \to \underline{H}$ is s.t.b a linear operator

if

- $L(\alpha x + \beta y) = \alpha L(x) + \beta L(y)$

- L is bounded if

$$\|Lx\| \leq K\|x\| \quad \forall x \in H.$$

$$\|L\| = \sup_{\|x\|=1} \|Lx\|.$$

- A linear operator is

  1. symmetric if $\langle Lx, y \rangle = \langle x, Ly \rangle$.
  2. non-neg definite if $\langle Lx, x \rangle \geq 0 \quad \forall x \in H$

③ pos-def if $\langle Lx, x\rangle > 0$ for all $x \neq 0$

<u>Defn</u>: A bounded linear operator L is s.t.b Hilbert-Schmidt if for some ONB

$$\|L\|_{HS}^2 := \sum_{j=1}^{\infty} \langle Le_j, Le_j\rangle < \infty$$

HS norm

Defn: A bounded linear operator L is s.t.b trace class if for a ONB, $\{e_j\}$:

$$Tr(L) = \sum_{j=1}^{\infty} \langle e_j, Le_j\rangle < \infty$$

Trace class $\Rightarrow$ HS $\Rightarrow$ Bounded

$\not\Leftarrow$ $\not\Leftarrow$

<u>Example</u> Consider $H = L^2([0,1])$.

$$\Rightarrow (Lx)(t) = \int k(t,s)\,x(s)\,ds$$

k is a kernel, and

$$\boxed{K := \iint k^2(t,s)\,ds\,dt < \infty}$$

$K < \infty \Rightarrow L$ is bounded

$\|L\| \leq K$

& L is Hilbert Schmidt

$\|L\|_{HS} = K^{\frac{1}{2}}$.

Eigenvalues & Eigenvectors:

λ is stb an eigenvalue of L if $\exists\, x \neq 0$

$Lx = \lambda x$.

x is stb a <u>eigenfunction</u>.

L symmetric $\Rightarrow$ $\lambda_i \in \mathbb{R}$

non-neg def $\Rightarrow$ $\lambda_i \geq 0$

pos def $\Rightarrow$ $\lambda_i > 0$

<u>Thm:</u> (HS theorem) If L symmetric, HS

Then $\exists$ a sequence of nonzero eigenvalues

$\lambda_1, \lambda_2, \ldots$ and assoc eigenfunctions $e_1, e_2, \ldots$

s.t.

$$x = \sum_{j=1}^{\infty} a_j e_j + v \quad \text{uniquely}$$

$L(v) = 0$.

Corollary: $$L x = \sum_{j=1}^{\infty} \lambda_j \langle x, e_j \rangle e_j$$

evalue   e function

$$L = \sum \lambda_j \, e_j \otimes e_j$$

Tensor: $(e_j \otimes e_j)(x) = \langle x, e_j \rangle e_j$

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2 Random Elements in a HS

Let X be a RV on $(H, \langle \cdot, \cdot \rangle)$.

What is $\mathbb{E}[X]$??

Construct an integral on H

If $\mathbb{E}\|X\| < \infty$ then $\mathbb{E}[X]$ is a Bochner integral and $\mathbb{E}[X]$ exists. strong

Consider $\mathbb{E}[\langle g, X\rangle] \approx \langle g, \mathbb{E}[X]\rangle$

If $\exists\, E \in H$ s.t. $\mathbb{E}\langle g, X\rangle = \langle g, E\rangle \quad \forall g \in H$

then define E to be the weak expectation.

If both strong & weak form exist, they must be equal.

$$\langle u, Kv\rangle = \mathbb{E}[\langle u, X-\mathbb{E}[X]\rangle\langle v, X-\mathbb{E}[X]\rangle]$$

K is the covariance operator.

$$K = \mathbb{E}[(X-\mathbb{E}[X])\otimes(X-\mathbb{E}[X])]$$

Gaussian RV on Hilbert Spaces.

Say that X on H is Gaussian,

if $\underbrace{\ell(X)}_{\text{a RV}}$ is Gaussian on $\mathbb{R}$ for all bounded linear functional ℓ.

In this case $\underbrace{\ell(X)}_{\langle g, X\rangle} \sim N(m_\ell, \sigma_\ell^2)$ by RRT

$$m_\ell = \ell(\mathbb{E}[X]) = \langle g, \mathbb{E}[X]\rangle$$

$$\sigma_\ell^2 = \langle g, \underline{K} g\rangle$$

$N(0, K)$ is a Gaussian measure if and only if K is a symmetric, non-negative definite, trace class operator on H.