## Lilly Why

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#### **RKHS**

RKHS theory is one of the most useful and elegant theories for mathematics and machine learning. It quantifies the model complexity by pointing out that the optimal solution from an infinity functional space is embedded into a finite dimensional subspace.

#### Personalized Intervention and Digital Health

Context: Digital technology will enable us to collect more individual

patient data.

Decision: The purpose of collecting these data is to generate

actionable insights.

Reward: The goal of these actionable insights is to maximize

individual patient's outcomes.



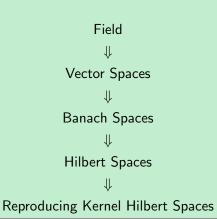
Can we leverage RKHS theory to enhance the solution for personalized intervention algorithms?

1 Introduction of Reproducing Kernel Hilbert Spaces

2 Personalized Intervention

## Lilly Introduction of RKHS

### Logic review



### Lilly Field: A field F is a structure $(F,+,\cdot,0,1)$

The following properties hold for a field:

- 2  $\forall \alpha, \beta, \gamma \in F, \alpha + (\beta + \gamma) = (\alpha + \beta) + \gamma$  (commutativity of addition)
- 3  $\forall \alpha, \beta \in F, \alpha \cdot \beta = \beta \cdot \alpha$  (commutativity of multiplication)
- **5**  $\forall \alpha, \beta, \gamma \in F, \alpha \cdot (\beta + \gamma) = \alpha \cdot \beta + \alpha \cdot \gamma$  (distributivity)
- **6**  $\exists$ 0 ∈ F,  $s.t. \forall \alpha \in F$ ,  $0 + \alpha = \alpha$  (additive identity)
- $\forall \alpha \in F, \exists -\alpha \in F, s.t.\alpha + (-\alpha) = 0 \text{ (additive inverse)}$
- ∃1 ∈ F, s.t. ∀α ∈ F, 1 · α = α (multiplication identity)

Example:  $\mathbb{Q}$ .

## Liley Vector Spaces: $+: V \times V \mapsto V, \cdot: F \times V \mapsto V$

The following properties hold for a vector space:

- 3  $\exists 0 \in V, s.t. \forall f \in V, 0 + f = f \text{ (additive identity)}$
- **6**  $\forall f \in V, \forall \alpha, \beta \in F, \alpha \cdot (\beta \cdot f) = (\alpha \cdot \beta) \cdot f$  (associativity of multiplication)
- **6**  $\forall f \in V, \forall \alpha, \beta \in F, (\alpha + \beta) \cdot f = \alpha \cdot f + \beta \cdot f$  (scalar distributivity)
- $\forall f, g \in V, \forall \alpha \in F, \alpha \cdot (f + g) = \alpha \cdot f + \alpha \cdot g$  (vector distributivity)
- 8  $\forall f \in V, \exists 1 \in F, 1 \cdot f = f \text{ (multiplicative identity)}$

Example:  $\mathbb{R}, \mathbb{R}^2, \mathbb{R}^{\mathbb{R}}, \mathbb{R}^{\mathcal{X}}, C(\mathcal{X})$ .

## Lilly Banach Spaces

### Definition (Banach Space)

A complete normed vector space is called a Banach Space.

### Normed Spaces

A vector space V is called a normed space if  $\forall f \in V$ ,  $\exists ||f|| \in \mathbb{R}$ , called the norm of u, such that

- ||f|| > 0 if  $f \neq 0$ , and ||f|| = 0 implies f = 0
- $||f + g|| \le ||f|| + ||g||$
- $\|\alpha f\| = |\alpha| \|f\|$ , where  $\alpha \in \mathbb{R}$

### Complete Vector Spaces

A vector space V is called complete if every Cauchy sequence in V convergent.

Example: Euclidean Spaces in  $\mathbb{R}^n$ ,  $L^p(V, \mathcal{F}, \mu)$  where  $p \in [1, +\infty) - \{2\}$ .

### Lilly Hilbert Spaces

### Definition (Hilbert Spaces)

A Hilbert space is a Banach space equipped with a dot product  $\langle \cdot, \cdot \rangle$ . The dot product operation satisfies the following properties,  $\forall f, g, h \in \mathcal{H}$  and  $\alpha \in F$ 

- Commutative:  $\langle f, g \rangle = \langle g, f \rangle$  and  $\langle f, g \rangle \in F$ .
- Associative:  $\langle \alpha \cdot f, g \rangle = a \cdot \langle f, g \rangle$
- Distributive:  $\langle f, g + h \rangle = \langle f, g \rangle + \langle f, h \rangle$

The norm of f is defined as  $||f|| = \sqrt{\langle f, f \rangle}$ .

Example:  $L^2(a, b)$ .

### Lilly Reproducing Kernel Hilbert Spaces(RKHS)

### Definition (RKHS)

A Hilbert space of real-valued functions  ${\cal H}$  is an RKHS if every evaluation functional is continuous.

#### **Evaluation functional**

Let  $\mathcal{H}$  be a Hilbert space of real-valued functions from  $\mathcal{X}$  to  $\mathbb{R}$ , i.e.  $\mathbb{R}^{\mathcal{X}}$  where  $\mathcal{X}$  is an arbitrary set. For a fixed  $x \in \mathcal{X}$ , the evaluation functional  $\mathcal{L}_x : \mathcal{H} \to \mathbb{R}$  is defined as,

$$\mathcal{L}_{x}f \triangleq f(x),$$

where  $f \in \mathcal{H}$ . Evaluation functionals are linear since,

$$\mathcal{L}_{x}(\alpha \cdot f + \beta \cdot g) = \alpha \cdot f(x) + \beta \cdot g(x) = \alpha \cdot \mathcal{L}_{x}f + \beta \cdot \mathcal{L}_{x}g.$$

## Lilly Reproducing Kernel

### Theorem (Riesz representation theorem)

Let T be a continuous linear functional on a Hilbert space  $\mathcal{H}$ . There exists a unique  $g_T \in \mathcal{H}$  such that  $Tf = \langle g_T, f \rangle, \forall f \in \mathcal{H}$ . The element  $g_T$  is called the representer of T.

#### Definition (Reproducing kernel)

Let  $K_x \in \mathcal{H}$  be a representer, and  $\langle K_x, f \rangle = f(x), \forall f \in \mathcal{H}$ . The symmetric bivariate function  $K(x,y) = \langle K_x, K_y \rangle = K_x(y) = K_y(x)$  is called the reproducing kernel (RK) of the space  $\mathcal{H}$  and it has the reproducing property  $\langle K(x,\cdot), f(\cdot) \rangle = f(x)$ .

### Theorem (Moore-Aronszajn theorem)

for every positive definite function  $K\langle\cdot,\cdot\rangle$  on  $\mathcal{X}\times\mathcal{X}$ , there exists a unique RKHS and vice versa.

### Liley Why RKHS Matters

A general class of regularization problems has the form,

$$\underset{f \in \mathcal{H}}{\operatorname{minimize}} \quad \left[ \sum_{i=1}^{n} L\{y_i, f(x_i)\} + \lambda J(f) \right],$$

where  $L(\cdot,\cdot)$  is a loss function,  $J(\cdot)$  is a penalty function, and  $\mathcal H$  is a space of functions on which  $J(\cdot)$  is defined. In particular, we have  $\mathcal H=\mathcal H_0\oplus\mathcal H_1$ , with the null space  $\mathcal H_0$  consisting of, for example, low degree polynomials in that elements do not get penalized. The penalty becomes  $J(f)=\|P_1f\|^2$ , where  $P_1$  is the orthogonal projection of f onto  $\mathcal H_1$ . If  $\mathcal H_1$  is a RKHS and  $L(\cdot,\cdot)$  is continuous and convex, the solution has the form,

$$f(x) = \sum_{j=1}^{m} \beta_j h_j(x) + \sum_{i=1}^{n} \alpha_i K(x, x_i),$$

where the first term represents an expansion in  $\mathcal{H}_0$ .

### Lilly Existence of Minimizer

A functional F(f) on a Hilbert space  $\mathcal{H}$  is said to be **convex** if  $\forall f, g \in \mathcal{H}, F\{\alpha \cdot f + (1-\alpha) \cdot g\} \leq \alpha F(f) + (1-\alpha)F(g), \forall \alpha \in (0,1)$ , and the convexity is strict if the equality holds only for f = g.

### Theorem (Existence)

Suppose L(f) is a continuous and convex functional in a Hilbert space  $\mathcal{H}$  and J(f) is a square (semi) norm in  $\mathcal{H}$  with a null space  $\mathcal{H}_0$  of finite dimension. If L(f) has a unique minimizer in  $\mathcal{H}_0$ , then  $L(f) + \lambda J(f)$  has a minimizer in  $\mathcal{H}$ .

Key to proof: Since  $L(f) + \lambda J(f)$  must has a minimizer in a closed rectangle set,

$$R_{\rho,\gamma} = \{f: f \in \mathcal{H}, J(f) \leq \rho, \|f - f_0\|_0 \leq \gamma\}, \forall \rho, \gamma, f \in \mathcal{H}\}$$

where  $f_0$  is the unique minimizer in  $\mathcal{H}_0$ , and  $\|\cdot\|_0$  is the norm on  $\mathcal{H}_0$ . If  $L(f) + \lambda J(f)$  doesn't have a minimizer in  $\mathcal{H}$ , the minimizer must be on the boundary of  $R_{\rho,\gamma}$ , by convexity, which cannot be true  $\forall \rho, \gamma$ .

### Lilly The Representer Theorem

### Theorem (The representer theorem)

Suppose L(f) is a continuous and convex functional in a Hilbert space  $\mathcal{H}$  and J(f) is a square (semi) norm in  $\mathcal{H}$  with a null space  $\mathcal{H}_0$  of finite dimension. If L(f) has a unique minimizer in  $\mathcal{H}_0$ , then  $L(f) + \lambda J(f)$  has a minimizer in  $\mathcal{H}$ , and

$$f(x) = \sum_{j=1}^{m} \beta_j h_j(x) + \sum_{i=1}^{n} \alpha_i K(x, x_i).$$

Key to proof: 
$$f = f_0 + f_K + f_\eta$$
 where  $f_0 \in \mathcal{H}_0$ ,  $f_K \in \mathcal{H}_K \triangleq \operatorname{span}\{K(x_1,\cdot), i=1,c\dots,n\}$  and  $f_\eta \in \mathcal{H} \ominus (\mathcal{H}_K \oplus \mathcal{H}_0)$ . Then, we have  $0 = \langle K(x_i,\cdot), f_\eta(\cdot) \rangle = f_\eta(x_i)$ . So,  $L\{(f_0 + f_K + f_\eta)(x_i)\} = L\{(f_0 + f_K)(x_i)\}$  and  $J(f) = J(f_K + f_\eta) = J(f_K) + J(f_\eta) > J(f_K)$ .

# Lilly Personalized Intervention